PORTLAND HARBOR RI/FS

BIOACCUMULATION MODELING REPORT

REVISED DRAFT

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June 19, 2015

Prepared for
The Lower Willamette Group

Prepared by
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WE-09-0003

RECOMMENDED FOR INCLUSION IN ADMINISTRATIVE RECORD

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Acronym	Definition
AOPC	area of potential concern
BEHP	bis(2-ethylhexyl) phthalate
BERA	baseline ecological risk assessment
BHHRA	baseline human health risk assessment
BIC	benthic invertebrate consumer
BIF	benthic invertebrate filter feeder
BSAF	biota-sediment accumulation factor
BSAR	biota-sediment accumulation regression
CAR	carp
CDD	chlorodibenzo-*p*-dioxin
CDF	chlorodibenzofuran
CF	correction factor
COC	chemical of concern
cPAH	carcinogenic polycyclic aromatic hydrocarbon
C_{sed} (or C_s)	sediment concentration
C_{tiss} (or C_t)	tissue concentration
~~**D**~~	~~detected~~
DDD	dichlorodiphenyldichloroethane
DDE	dichlorodiphenyldichloroethylene
DDT	dichlorodiphenyltrichloroethane
DF	detection frequency
DL	detection limit
DOC	dissolved organic carbon
dw	dry weight
EIC	epibenthic invertebrate consumer
EPA	US Environmental Protection Agency
ERA	ecological risk assessment
FWM	food web model
HCH	hexachlorocyclohexane
HHRA	human health risk assessment
HQ	hazard quotient
iPRG	initial preliminary remediation goal
ISD	insufficient data to develop a BSAR

Acronym	Definition
K_M	metabolic rate constant
K_{OW}	octanol-water partition coefficient
LSS	largescale sucker
LWG	Lower Willamette Group
~~LSS~~	~~largescale sucker~~
NA	not applicable
NC	model for TEQ conversion did not pass screening requirements
~~ND~~	~~not detected~~
ND	no data
NE	not evaluated
NJ	tentatively identified, detected concentration is approximate
NLOC	non-lipid organic carbon
NLOM	non-lipid organic matter
NM	no model developed
NPM	northern pikeminnow
NTD	no tissue data, tissue not analyzed for this chemical, and thus no BSAF could be developed
OC	organic carbon
ODEQ	Oregon Department of Environmental Quality
PAH	polycyclic aromatic hydrocarbon
PCB	polychlorinated biphenyl
PCDD	polychlorinated dibenzo-*p*-dioxin
PDCF	polychlorinated dibenzofuran
PeCDF	pentachlorodibenzofuran
PRG	preliminary remediation goal
r^2	coefficient of determination
RI/FS	remedial investigation/feasibility study
RL	reporting limit
RM	river mile
SCL	sculpin
SCRA	site characterization and risk assessment
SD	standard deviation
SMB	smallmouth bass
SPAF	species predictive accuracy factor
SVOC	semivolatile organic compound
SWAC	spatially weighted average concentration

Acronym	Definition
TBT	tributyltin
~~**TCDD**~~	~~tetrachlorodibenzo-p-dioxin~~
~~**TEF**~~	~~toxic equivalency factor~~
TEQ	toxic equivalent
total DDx	sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE and 4,4′-DDT)
TRV	toxicity reference value
TSS	total suspended solids
USACE	US Army Corps of Engineers
VBA	Visual Basic for Applications®
ww	wet weight
XAD	XAD – Infiltrex™ system with XAD resin column

1.0 INTRODUCTION

Bioaccumulation models were developed for Portland Harbor primarily for producing sediment preliminary remediation goals (PRGs) for bioaccumulative chemicals of concern (COCs). PRGs will be used to identify areas of potential concern (AOPCs) and, in conjunction with fate and transport models, to evaluate different remedial options.

The basic objective of this sediment PRG model is to estimate the sediment concentration at which a threshold tissue concentration (i.e., maximum acceptable concentration of a COC in tissue) would be reached, given some assumptions about other chemical sources (e.g., lateral or upstream chemical inputs). In the context of this report, that estimated sediment concentration is the sediment PRG. In general, the PRG is a spatially weighted average concentration (SWAC) over an assumed exposure area. When the average tissue concentration in the exposure area equals the tissue threshold, the average sediment concentration for that area equals the PRG.

There are two basic modeling approaches for developing sediment PRGs: statistical and mechanistic. Barber (2008) provides a technical discussion of these approaches for bioaccumulative organic chemicals. The Lower Willamette Group (LWG) and US Environmental Protection Agency (EPA) negotiated the sediment PRG modeling approach for the Portland Harbor remedial investigation/feasibility study (RI/FS) over several years. An agreement was reached at a June 6, 2006, meeting between EPA and the LWG to use a mechanistic bioaccumulation model (Arnot and Gobas 2004) for polychlorinated biphenyls (PCBs), dichlorodiphenyltrichloroethanes (DDTs), and dioxin-like chemicals. Other persistent hydrophobic organic chemicals were not identified for mechanistic bioaccumulation modeling at the time because detection frequencies were low in the sediment and tissue chemistry data that were then available (only Round 1 and 2 data). The June 6, 2006, agreement also stipulated that the LWG would attempt to develop statistical models for any other COCs in Portland Harbor, and if successful, use them to develop PRGs.

From available Round 1 and Round 2 data, bioaccumulation models were developed and used to generate initial PRGs for initial chemicals of concern in the Round 2 report (Integral et al. 2007). EPA's August 8, 2008, comments on the bioaccumulation modeling appendix of the Round 2 report reiterated the "longstanding agreement between EPA and the LWG to use the Arnot and Gobas food web model (FWM) at Portland Harbor" (EPA 2008b). With the Round 3 sampling program, which generated substantially more tissue and water chemistry data than were previously available, there are sufficient data to use the Arnot and Gobas model for other organochlorine pesticides besides DDTs. Using data from Rounds 1-3 sampling efforts, the Arnot and Gobas model was used for all organochlorine pesticide, PCB, and polychlorinated dibenzo-*p*-dioxin (PCDD)/polychlorinated dibenzofuran (PCDF) COCs. Statistical models (biota-sediment accumulation regressions/ factors [BSAR/Fs]) were used for other COCs as statistically appropriate.

This report describes the development of the bioaccumulation models for COCs identified in the baseline human health risk assessment (BHHRA) (Kennedy/Jenks 2013) and baseline ecological risk assessment (BERA) (Windward 2013), and the application of these bioaccumulation models to generate PRGs. This report first provides the chemicals to be modeled, then a discussion of general methodology common to the statistical and mechanistic bioaccumulation models, followed by development and application of statistical models (BSAR/Fs), and finally mechanistic model development and application.

2.0 CHEMICALS MODELED

Tables 2-1 and 2-2 list the preliminary human health and ecological COCs and indicate whether development of the mechanistic model or a BSAR/F was attempted for use in early PRG development. BSAR/F development is presented in Section 4.0 and the mechanistic model is described in Section 5.0. Mechanistic modeling is the preferred method for developing PRGs because it accounts explicitly for water contribution to COC concentrations in tissue and therefore can be used to analyze the relative contributions of sediment contamination and water contamination to COC concentrations in tissue. Further, the mechanistic model can be used to estimate beyond the range of available data (e.g., to predict tissue COC concentrations lower than were found in collected fish samples), whereas BSAR/Fs should be used only to interpolate within the range of data used to develop them (Neter et al. 1990).

The mechanistic model is appropriate for hydrophobic organic chemicals (Arnot and Gobas 2004). If a chemical was identified as an ecological COC or human health COC based on risk associated with any one species and the mechanistic model could not be applied for a given chemical-species combination, BSAR/F development for that chemical-species combination was attempted (e.g., metals and polycyclic aromatic hydrocarbons [PAHs] for all species). Early PRGs were not developed for all chemical-species combinations, but for only those associated with risk estimates of concern (i.e., hazard quotients [HQs] > 1 or upper-bound cancer risk estimates greater than 1 in 1 million) based on concentrations in tissue of the receptor itself or of its prey or dietary items. The COCs for the human and ecological risk assessments are listed in Tables 2-1 and 2-2. The relative importance of these COCs (i.e., their contribution to risk) varies greatly. For human health, the overwhelming majority of risk on a Study Area-wide basis is attributable to PCBs, followed distantly by dioxins and then by DDTs. For ecological health, PCBs were the chemical group that contributed the most to ecological risks on a Study Area-wide basis. Thus, the mechanistic model is appropriate for the chemical group associated with the greatest proportion of risk (PCBs) and several other COCs.

Table 2-1. Modeling Methods Attempted for Development of Early PRGs for Ecological COCs

	Invertebrates					Fish							
COC	**Clams**	**Crayfish**	**Multi-plates**	**Mussels**	**Worms**	**Brown Bullhead**	**Carp**	**Lamprey**	**Largescale Sucker**	**Northern Pikeminnow**	**Pea-mouth**	**Sculpin**	**Smallmouth Bass**
Metals													
Arsenic					BSAR								
Cadmium	BSAR		NA[a]		BSAR							BSAR	
Copper	BSAR	BSAR	NA[a]		BSAR		BSAF	BSAF	BSAF	BSAF	BSAR	BSAR	
Lead		BSAR				BSAF	BSAF		BSAF	BSAF	BSAR	BSAR	BSAR
Mercury							BSAF		BSAF	BSAF	BSAR		
Zinc	BSAR			NA[a]	BSAR								
PAHs													
Benzo(a)pyrene					BSAR								
Phth~~l~~alates													
BEHP	BSAR												
Dibutyl phthalate	BSAR												
Butyltins													
TBT	BSAR	BSAR			BSAR		BSAF					BSAR	
PCBs													
Total PCBs	Mech	Mech			Mech	Mech	Mech		Mech	Mech	Mech	Mech	Mech
~~PCB TEQ (birds)[b]~~					~~Mech~~	~~Mech~~	~~Mech~~		~~Mech~~	~~Mech~~			~~Mech~~
~~PCB TEQ (mammal)[b]~~		~~Mech~~					~~Mech~~					~~Mech~~	~~Mech~~
~~**Dioxins and Furans**~~													
~~Dioxin TEQ (birds)[c]~~					~~Mech~~	~~Mech~~	~~Mech~~		~~Mech~~	~~Mech~~			~~Mech~~
~~Dioxin TEQ (mammal)[c]~~		~~Mech~~										~~Mech~~	~~Mech~~

Table 2-1. Modeling Methods Attempted for Development of Early PRGs for Ecological COCs

	Invertebrates					Fish							
COC	Clams	Crayfish	Multi-plates	Mussels	Worms	Brown Bullhead	Carp	Lamprey	Largescale Sucker	Northern Pikeminnow	Pea-mouth	Sculpin	Smallmouth Bass
Pesticides													
Aldrin					Mech								
Sum DDE						Mech	Mech		Mech	Mech	Mech		Mech
Total DDx	Mech				Mech							Mech	

Note : Total TEQs (the sum of the PCB TEQ and the dioxin TEQ for birds and mammals) were calculated in the BERA, but no PRGs will be calculated for total TEQ. ~~(PRGs are available for both the PCB TEQ and dioxin TEQ)~~.

[a] No BSAF or BSAR was developed for these species because their tissue contamination is expected to be driven by water exposure (rather than sediment exposure)

~~[b] The surrogate for PCB TEQ (birds) is PCB 77 and the surrogate for PCB TEQ (mammals) is PCB 126.~~

~~[c] The surrogate for dioxin/furan TEQ (birds and mammals) is 2,3,4,7,8-PeCDF~~

BEHP – bis(2-ethylhexyl) phthalate
BERA – baseline ecological risk assessment
BSAF – biota-sediment accumulation factor
BSAR – biota-sediment accumulation regression
COC – chemical of concern
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
Mech – mechanistic model
NA – not applicable
PAH – polycyclic aromatic hydrocarbon
PCB – polychlorinated biphenyl
~~PeCDF – pentachlorodibenzofuran~~
PRG – preliminary remediation goal
TBT – tributyltin
TEQ – toxic equivalent
total DDx – sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE, and 4,4′-DDT)

Table 2-2. Modeling Methods Attempted for Development of Early PRGs for Human Health COCs

COC	Clams	Crayfish	Black Crappie	Brown Bullhead	Carp	Smallmouth Bass
Metals						
Antimony			BSAF	BSAF	BSAF	BSAR
Arsenic	BSAR	BSAR	BSAF	BSAF	BSAF	BSAR
Lead			BSAF	BSAF	BSAF	BSAR
Mercury			BSAF	BSAF	BSAF	BSAR
Selenium			BSAF	BSAF	BSAF	BSAR
Zinc			BSAF	BSAF	BSAF	BSAR
PAHs						
Benzo(a)anthracene	BSAR	BSAR	BSAF	BSAF	BSAF	BSAR
Benzo(a)pyrene	BSAR	BSAR	BSAF	BSAF	BSAF	BSAR
Benzo(b)fluoranthene	BSAR	BSAR				
Benzo(k)fluoranthene	BSAR	BSAR				
Chrysene	BSAR	BSAR				
Dibenzo(a,h)anthracene	BSAR	BSAR	BSAF	BSAF	BSAF	BSAR
Indeno(1,2,3-cd)pyrene	BSAR	BSAR				
Total cPAHs	BSAR	BSAR	BSAF	BSAF	BSAF	BSAR
Phthalates						
BEHP			BSAF	BSAF	BSAF	BSAR
SVOCs						
Hexachlorobenzene	BSAR	BSAR	BSAF	BSAF	BSAF	BSAR
Pentachlorophenol		BSAR				
PCBs						
Total PCBs	Mech	Mech	Mech	Mech	Mech	Mech
~~PCB TEQ (mammals)[a]~~	~~Mech~~	~~Mech~~	~~Mech~~	~~Mech~~	~~Mech~~	~~Mech~~
~~**Dioxins and Furans**~~						
~~Dioxin/furan TEQ (mammals)[b]~~	~~Mech~~	~~Mech~~	~~Mech~~	~~Mech~~	~~Mech~~	~~Mech~~
Pesticides						
Aldrin	Mech	Mech	Mech	Mech	Mech	Mech
alpha-HCH			Mech	Mech	Mech	Mech
beta-HCH			Mech	Mech	Mech	Mech

Table 2-2. Modeling Methods Attempted for Development of Early PRGs for Human Health COCs

COC	Clams	Crayfish	Black Crappie	Brown Bullhead	Carp	Smallmouth Bass
Dieldrin	Mech	Mech	Mech	Mech	Mech	Mech
gamma-HCH			Mech	Mech	Mech	Mech
Heptachlor			Mech	Mech	Mech	Mech
Heptachlor epoxide	Mech	Mech	Mech	Mech	Mech	Mech
Sum DDD	Mech	Mech	Mech	Mech	Mech	Mech
Sum DDE	Mech	Mech	Mech	Mech	Mech	Mech
Sum DDT	Mech	Mech	Mech	Mech	Mech	Mech
Total chlordane			Mech	Mech	Mech	Mech

~~[a] The surrogate for PCB TEQ (mammals) is PCB 126.~~
~~[b] The surrogate for dioxin/furan TEQ (mammals) is 2,3,4,7,8-PeCDF.~~

BEHP – bis(2-ethylhexyl) phthalate
BSAF – biota-sediment accumulation factor
BSAR – biota-sediment accumulation regression
COC – chemical of concern
cPAH – carcinogenic polycyclic aromatic hydrocarbon
DDD – dichlorodiphenyldichloroethane
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
HCH – hexachlorocyclohexane
Mech – mechanistic model
PAH – polycyclic aromatic hydrocarbon
PCB – polychlorinated biphenyl
~~PeCDF – pentachlorodebenzofuran~~
PRG – preliminary remediation goal
SVOC – semivolatile organic compound
~~TEQ – toxic equivalent~~

3.0 GENERAL METHODOLOGY

The mechanistic model was used for early PRG development because it accounts for water contribution explicitly and because it can be used to estimate beyond the range of the data from which it was developed (as was necessary for development of several early PRGs). The size of the available datasets for model development is larger than was the case for previous efforts (specifically, the addition of a large number of tissue samples from Round 3), allowing the mechanistic model to be applied to more COCs than was possible in the Round 2 report (Integral et al. 2007). The mechanistic model here is used for PCBs, dioxins, and pesticides. The mechanistic model (Arnot and Gobas 2004) was designed for hydrophobic organic chemicals, and BSAR/Fs were used to model the remaining COCs (metals, PAHs,[1] semivolatile organic compounds [SVOCs], phthalates, and tributyltin [TBT]).

The Arnot and Gobas model explicitly accounts for the kinetics of chemical uptake and loss/dilution based on a mechanistic understanding of these processes. Because it is mechanistic, the model is appropriate for extrapolating beyond the empirically observed conditions in Portland Harbor, for example to project possible future conditions, to explore different assumptions about source terms (e.g., sediment versus lateral and upstream sources), or to calculate PRGs that fall outside the range of observed sediment concentrations. The fact that the Arnot and Gobas model is mechanistic also means that it can be calibrated to the data for a subset of chemicals and aquatic species and then "validated" with the data for other combinations of chemicals and species. The Arnot and Gobas model requires information about more parameters than do BSAR/Fs (e.g., water chemistry data, species-specific lipid content and body weights) and is appropriate for some hydrophobic organic chemicals only.

The appropriate uses of statistical models are more limited relative to mechanistic models (because they lack power to predict beyond the range of the data used to build the model or to predict when the conditions underlying the contributing data change). However, statistical models are the only option when the processes affecting bioaccumulation are not adequately understood. For example, modeling the fate of bioaccumulative metals generally requires a sophisticated, site-specific understanding of biogeochemistry that is often not readily available.

Model development was attempted for each COC-receptor pair (or dietary prey species). The models that were developed were used to estimate early PRGs. To develop sediment PRGs, the models were essentially run backwards to estimate the sediment concentration that would be associated with a specified target tissue concentration (based on the tissue

[1] PAHs are poor candidates for application of the mechanistic model because they are highly metabolized, and rates of metabolism by different species are not well defined.

toxicity reference value [TRV] or acceptable tissue concentration for a consumed species). The resulting sediment concentrations were used as early PRGs.

While the methodology and logic behind the development of mechanistic and statistical bioaccumulation models are quite different, numerous general methodologies are the same for both approaches. This section describes the methodology for dealing with chemical mixtures with toxicity equivalents, data preparation issues, and exposure area considerations, all of which are applicable to both mechanistic and statistical models.

3.1 DATASET SUMS AND TOTALS CALCULATIONS AND DATA QUALITY ISSUES

This section describes the available data and the approaches for calculating totals used for BSAR/Fs and the mechanistic model. Previous modeling efforts (Integral et al. 2007; Windward 2005, 2004) included data for tissue, sediment, and water generated during Round 1 and Round 2 fieldwork. This effort includes Round 3 data for these media. Round 3 data added 74 tissue chemistry samples to the 241 available from Rounds 1 and 2 and 189 water chemistry samples to the 101 available previously; 193 sediment samples were added in Round 3 to the 1,469 previous available for the BERA dataset (Windward 2013).

3.1.1 Total PCBs

For the sediment and tissue dataset, total PCBs was based on the sum of PCB congeners when those data were available and on the sum of PCB Aroclors when no congener data were available. For the water dataset, total PCBs was calculated as the sum of PCB congeners, as described in Section 5.3.5.2.1. A chemical was determined to be “present” at the site (Study Area) if it was detected at least once in a given medium (and tissue type). If a PCB congener or Aroclor determined to be “present” was not detected in a particular sample (but other congeners or Aroclors were detected), then one-half the detection limit (DL) was used for that congener or Aroclor in the total. If no analytes (congeners or Aroclors) were detected in a given sample, then the highest DL (for Aroclors or congeners, respectively) was used to estimate the total concentration.

~~3.1.2 Toxic Equivalents~~

~~Toxic equivalents (TEQs) for dioxin-like PCB congeners and for polychlorinated dibenzo-*p*-dioxins and dibenzofurans were calculated using the same methodology as was used in the BERA. A TEQ is the weighted sum of concentrations of dioxin-like congeners, where the weights reflect the toxicity of each constituent relative to the most toxic constituent (2,3,7,8-tetrachlorodibenzo-*p*- dioxin [TCDD]). Toxicity equivalency factors (TEFs) are based on the World Health Organization values for fish and birds (Van den Berg et al. 1998) and mammals (Van den Berg et al. 2006), as presented in Tables 3-1 and 3-2. TEQs were calculated if at least one TEQ constituent for a given sample was detected using the following method:~~

- ~~If an analyte was detected (D), the concentration was multiplied by the TEF in the sum.~~
- ~~If an analyte was not detected (ND) but had been detected in another sample in the BERA dataset, one-half the DL was multiplied by the TEF in the sum.~~
- ~~If an analyte was ND and had not been detected in any other sample in the BERA dataset, the value of zero was used in sum.~~
- ~~If all analytes used to create a TEQ were ND, the maximum toxicity-weighted DL was reported as the TEQ.~~

~~Table 3-1. Dioxin-Like PCB Congener TEFs~~

~~Congener Number~~	~~TEF Value (unitless)~~	
	~~Birds~~[a]	~~Mammals~~[b]
~~PCB 77~~	~~0.05~~	~~0.0001~~
~~PCB 81~~	~~0.1~~	~~0.0003~~
~~PCB 105~~	~~0.0001~~	~~0.0003~~
~~PCB 114~~	~~0.0001~~	~~0.0003~~
~~PCB 118~~	~~0.00001~~	~~0.0003~~
~~PCB 123~~	~~0.00001~~	~~0.0003~~
~~PCB 126~~	~~0.1~~	~~0.1~~
~~PCB 156~~	~~0.0001~~	~~0.0003~~
~~PCB 157~~	~~0.0001~~	~~0.0003~~
~~PCB 167~~	~~0.00001~~	~~0.0003~~
~~PCB 169~~	~~0.001~~	~~0.03~~
~~PCB 189~~	~~0.00001~~	~~0.0003~~

[a] ~~Bird TEFs are based on Van den Berg et al. (1998).~~
[b] ~~Mammal TEFs are based on Van den Berg et al. (2006).~~
~~PCB – polychlorinated biphenyl~~
~~TEF – toxic equivalency factor~~

~~**Table 3-2. Dioxin and Furan TEFs**~~

~~Dioxin and Furan Congeners~~	~~TEF Value (unitless)~~	
	~~Birds[a]~~	~~Mammals[b]~~
~~2,3,7,8-Tetrachlorodibenzo-*p*-dioxin~~	~~1~~	~~1~~
~~1,2,3,7,8-Pentachlorodibenzo-*p*-dioxin~~	~~1~~	~~1~~
~~1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin~~	~~0.05~~	~~0.1~~
~~1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin~~	~~0.01~~	~~0.1~~
~~1,2,3,7,8,9-Hexachlorodibenzo-*p*-dioxin~~	~~0.1~~	~~0.1~~
~~1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin~~	~~< 0.001~~	~~0.01~~
~~Octachlorodibenzodioxin~~	~~0.0001~~	~~0.0003~~
~~2,3,7,8-Tetrachlorodibenzofuran~~	~~1~~	~~0.1~~
~~1,2,3,7,8-Pentachlorodibenzofuran~~	~~0.1~~	~~0.03~~
~~2,3,4,7,8-Pentachlorodibenzofuran~~	~~1~~	~~0.3~~
~~1,2,3,4,7,8-Hexachlorodibenzofuran~~	~~0.1~~	~~0.1~~
~~1,2,3,6,7,8-Hexachlorodibenzofuran~~	~~0.1~~	~~0.1~~
~~1,2,3,7,8,9-Hexachlorodibenzofuran~~	~~0.1~~	~~0.1~~
~~2,3,4,6,7,8-Hexachlorodibenzofuran~~	~~0.1~~	~~0.1~~
~~1,2,3,4,6,7,8-Heptachlorodibenzofuran~~	~~0.01~~	~~0.01~~
~~1,2,3,4,7,8,9-Heptachlorodibenzofuran~~	~~0.01~~	~~0.01~~
~~Octachlorodibenzofuran~~	~~0.0001~~	~~0.0003~~

[a] ~~Bird TEFs are based on Van den Berg et al. (1998).~~
[b] ~~Mammal TEFs are based on Van den Berg et al. (2006).~~
~~TEF – toxic equivalency factor~~

~~Regardless of the approach used for treatment of ND analytes (e.g., use of one-half the DL, use of zero, or use of the DL in sums) most estimates of TEQ were similar because the DLs for NDs were generally low compared to detected concentrations.~~

~~The rationale for using TEFs is based on evidence that there is a common mechanism of toxicity for certain dioxins, furans, and PCB congeners, which involves binding to the aryl hydrocarbon receptor. Data on the relative binding affinity of particular PCB congeners compared to 2,3,7,8-TCDD are available from *in vivo* and *in vitro* studies. These data have been used to derive TEFs for PCB congeners that show structural similarity to dioxins, bind to the aryl hydrocarbon receptor, and elicit dioxin-specific biochemical and toxic responses.~~

3.1.2~~3~~ Total DDx

Total DDx (i.e., the sum of all dichlorodiphenyldichloroethane [DDD], dichlorodiphenyldichloroethylene [DDE], and DDT isomers together), sum DDD (the sum of the 2,2′ and 2,4′ isomers of DDD), sum DDE (the sum of the 2,2′ and 2,4′ isomers of DDE) and sum DDT (the sum of the 2,2′ and 2,4′ isomers of DDT) were calculated as the sum of the detected concentrations and one-half the DL for undetected isomers. If no DDT isomers for a sum or total were detected, then that sum or total was equal to the highest DL of the isomers included in the sum or total. Round 1 tissue samples were analyzed for pesticides using EPA method SW8081.

With the exception of whole-body juvenile Chinook salmon, which were also analyzed using EPA method SW8081, all Round 2 and 3 tissue samples were analyzed for pesticides by AXYS Analytical Services using a high-resolution analytical method (MLA-028) to reduce DLs. Thus the detection frequency and DLs for DDTs in tissue were improved significantly between these rounds of sampling. Several other pesticides also had elevated DLs in Round 1 (compared to Rounds 2 and 3) as well.

The improved analytical method used for the Round 2 and 3 data had the largest impact on the average crayfish and average sculpin DDT tissue concentrations. For example, the Round 1 dataset for crayfish for 4,4′-DDT (8 of 27 samples detected) had an average concentration approximately 80 times that of the Round 3 dataset (1 of 5 samples detected). While both of these datasets had low detection frequencies, the average reporting limit for the Round 1 dataset was 1.9 µg/kg dry weight (dw) and that for the Round 3 dataset was 0.019 µg/kg dw. While the influence of these higher reporting limits may have been less for other species or chemicals, the example highlights the uncertainties surrounding these data and the benefit of the additional Round 3 data with improved detection limits for pesticides.

~~3.2 APPROACH FOR CHEMICAL MIXTURES WITH TOXICITY EQUIVALENTS~~

~~The TEQ in a particular medium (e.g., tissue) represents the concentration and toxicity of the mixture of congeners present. The individual congeners have different toxicities (as represented by their TEFs) and bioaccumulate differently from one another because of their different physical properties. Therefore, a single congener that was strongly correlated with the TEQ was selected as a surrogate that could be used to model the bioaccumulation of the entire suite of compounds. Surrogate selection and development of regression relationships to relate the surrogates to the TEQ are described in detail in Appendix A. Briefly, data on TEQ concentrations and on concentrations of the TEQ congeners (unadjusted for toxicity) were evaluated to identify an individual surrogate congener for each TEQ. The following surrogates were selected:~~

- ~~PCB 77 for the bird PCB TEQ~~
- ~~PCB 126 for the mammal PCB TEQ~~
- ~~2,3,4,7,8-pentachlorodibenzofuran for the bird PCDD/F TEQ~~
- ~~2,3,4,7,8-pentachlorodibenzofuran for the mammal PCDD/F TEQ~~

~~The regression equations relating each of these congeners to its respective TEQ are presented in Appendix A for each species. These equations were used to calculate PRGs for PCDD/Fs and dioxin-like PCBs in terms of their surrogate congener concentrations. TEQ PRG development is discussed further in Section 4.4.~~

3.2~~3~~ EXPOSURE AREA CONSIDERATIONS

Bioaccumulation modeling required assumptions about exposure areas of the species modeled. These assumptions affect PRGs derived from the models, as well as the scales at which the PRGs may be applied.

3.2~~3~~.1 Species with Home Ranges Smaller than the Site

For benthic invertebrate BSAR development and some mechanistic model applications at spatial scales smaller than site-wide, each tissue sample included had a paired co-located sediment sample (i.e., the sediment chemical concentration in the co-located sediment sample was assumed to describe the sediment exposure for a given tissue sample).

Co-located sediment samples were used to estimate sediment exposure concentrations for benthic invertebrates (Section 3.3.2). Study Area-wide average sediment concentrations were used to estimate exposure for wide-ranging fish species. Sediment exposure areas for sculpin and smallmouth bass were larger than a single point and smaller than the entire Study Area. For these two species, methods were developed to estimate intermediate-scale sediment exposure concentrations. These approaches are described in Section 3.3.3.

3.2~~3~~.2 Data Preparation for Benthic Invertebrates

The BERA datasets[2] for the receptor-chemical pairs presented in Tables 2-1 and 2-2 were used to develop BSARs. Empirical sediment chemical concentrations (expressed as dry weight- and organic carbon (OC)-normalized concentrations) and co-located tissue concentrations (expressed as wet weight (ww)- and lipid-normalized concentrations) were used. Up to 40 co-located sediment and tissue data pairs were evaluated for field-collected clams and up to 28 pairs were evaluated for crayfish. Up to 35 co-located sediment and tissue data pairs were evaluated for clams and worms exposed to Study Area sediments in 28-day laboratory bioaccumulation tests.

Per EPA direction (EPA 2008c), the concentrations of neutral organic COCs (i.e., butyltins, PCBs, phthalates, and pesticides) measured in laboratory clam and laboratory worm tissue were adjusted to estimate steady-state concentrations. The process used for the adjustment is described in the US Army Corps of Engineers' (USACE) *Inland Testing Manual* (EPA and USACE 1998), based on McFarland (1994). The rationale for the adjustment is that a 28-day laboratory exposure period is not sufficiently long for all neutral organics to reach steady-state tissue concentrations. Because field-collected clam data were available, the data from laboratory-exposed clam were not used for bioaccumulation modeling. The field clams were exposed to Study Area sediment and water, whereas the laboratory clams were exposed to sediment collected from the Study Area but not Study Area water. The laboratory worms were also only exposed to Study Area sediment, but because there was no better alternative for estimating bioaccumulation for worms, these data were used for bioaccumulation modeling.

[2] The BERA dataset is defined in Section 4 of Appendix H of the remedial investigation report.

Any co-located data pair with non-detected tissue or sediment concentrations was removed from the BSAR analysis, so that only pairs of detected sediment and detected tissue concentrations were used in BSAR development per Burkhard (2006). As discussed in Section 4.0, for all non-metals, sediment chemical concentrations were normalized based on OC content, and tissue chemical concentrations were normalized based on lipid content to account for the partitioning of these chemicals. No adjustments were made to sediment and tissue chemical concentrations for metals.

3.2~~3~~.3 Data Preparation for Smallmouth Bass and Sculpin

In the BERA dataset, 39 composite tissue samples were analyzed for whole-body sculpin and 32 composite tissue samples were analyzed for whole-body smallmouth bass. Special methods for describing exposure areas were developed for sculpin and bass. These exposure areas represent the foraging areas of the target species and their prey.

For sculpin, the exposure area selected was a circle of 0.1-mile radius centered on the sculpin composite sample centroid. Foraging ranges reported in the literature support small home ranges for sculpin. Sculpin movements of over 200 ft have been reported in the literature (Hill and Grossman 1987; Natsumeda 1998, 1999, 2001; Petty and Grossman 2004; Cunjak et al. 2005). An exposure radius of approximately 0.1 mile (500 ft) was assumed to be representative of the foraging area of the sculpin and their prey in a given composite sample and to approximate the area over which the individuals in a composite sample were collected. The SWAC for that circular area was used as the sediment exposure concentration for the co-located sculpin composite. Natural neighbors interpolation[3] (de Smith et al. 2008) of the BERA surface sediment dataset was used to estimate the SWAC that was assigned to each composite sculpin sample. The resultant SWACs are presented in Appendix ~~B~~A.

For smallmouth bass, the exposure reach for each composite sample was assumed to be a 1-mile length of the river. Foraging ranges and movements reported in the literature and in region-specific studies have supported home ranges for smallmouth bass that are smaller than the entire length of the Study Area. Pribyl et al. (2005) conducted a study from 2000 to 2003 in which the movement of predatory resident fish (including smallmouth bass) in the Lower Willamette River was tracked using radio-tagged fish. Radio-tagged smallmouth bass tended to stay near release points, and the median of the maximum distance traveled over the tracking period by smallmouth bass was 2.3 km (1.4 miles) from the release site. Most smallmouth bass stayed within 0.4 km (0.25 mile) of their release points in the 1-

[3] The natural neighbors interpolation algorithm is built into ArcGIS software. Natural neighbors interpolation calculates the value for each cell by adding the cell center coordinates to the actual set of sampling locations, finding its hypothetical Thiessen polygon in relation to them, and overlaying this hypothetical polygon on the actual Thiessen polygons for the sample set. The calculated cell value is a mean of the neighboring sampled values weighted proportionally to the area that each actual sample polygon occupies within the cell's hypothetical polygon (de Smith et al. 2008).

month post-release period. An exposure area of approximately 1 mile was assumed to be representative of the foraging range of the smallmouth bass in a given composite.

Because it was unknown whether the smallmouth bass would forage upstream or downstream from their collection point, 1-river-mile (RM) exposure areas at 0.1-mile increments were evaluated ranging from 1 mile upstream to 1 mile downstream of the collection location of each smallmouth bass in a given composite.[4] Thus there were up to 10 exposure estimates (each being a SWAC covering 1 RM) for each collection location. The SWACs for all the fish within a composite were then averaged. Due to the scatter or closeness of the individual fish collected for each composite tissue sample and the upstream and downstream boundaries of the site (exposure was not estimated for areas beyond study boundaries), the number of 1-mile exposure areas averaged for each composite varied. The 1-mile exposure areas had boundaries perpendicular to the river course; SWACs for these areas were calculated from natural neighbors interpolations and are provided in Appendix ~~B~~A. Again, the sediment chemistry data for the natural neighbor interpolation came from the BERA dataset.

The sediment data used to generate SWACs were based on the BERA dataset, which included a subset of data from the site characterization and risk assessment (SCRA) database. Only those data in the SCRA database that were of acceptable data quality for risk evaluation (Category 1/QA2) were included in the BERA dataset, as per the programmatic work plan (Integral et al. 2004). Surface sediment in the BERA dataset included data collected within the top 30.5 cm of the sediment horizon and located within the Study Area (RM 1.9 to RM 11.8), excluding Round 1 beach sediment sampled for use in the BHHRA. Sediment natural attenuation cores collected by LWG for nature and extent studies were also not included in the BERA dataset because multiple depth intervals in small increments (as small as 4 cm) were collected within the 0-to-30.5-cm surface sediment depth horizon.

For geographic information system mapping, surface sediment concentrations qualified as non-detects were assigned one-half the RL value. Only those stations with reported results (detect or non-detect data) were included in the set of points for generating natural neighbors for the SWAC calculation.

3.2~~3~~.4 General Approach for Large-Home-Range Species

Lower Willamette River telemetry studies (Friesen 2005; Pribyl et al. 2005) support the assumption that black crappie, carp, northern pikeminnow, largescale sucker, and brown bullhead range over areas larger than the Study Area; Study Area-wide SWACs were used to estimate sediment exposure concentrations for those fish species. The same process and sediment dataset was used for developing SWACs for large-home-range species as was used for sculpin and smallmouth bass.

[4] The study area (RM 1.9 to 11.8) was stratified by 0.1-mile increments, and a SWAC based on natural neighbor interpolation was calculated for each RM.

4.0 EVALUATION OF BSARS AND BSAFS

PRGs, and therefore BSAR/Fs, were developed for only chemical-exposure scenario combinations that were identified as COCs. For example, a chemical that could not be modeled mechanistically might be a COC based on human consumption of clams but not a COC for human consumption of fish or for any ecological risk scenario. In such a case, the development of a BSAR/F might be attempted only for clams but not for any other species. For chemicals for which the mechanistic model could not be applied (see Tables 2-1 and 2-2), BSAR/Fs were used to estimate PRGs when a linear relationship between co-located[5] sediment and tissue concentrations could be established on the basis of data collected for the baseline risk assessments. The BSAR assumes a relationship between the concentration of a bioaccumulative chemical in sediment and that measured in tissue. Frequently, the relationship between tissue and sediment concentrations is calculated as the ratio of tissue and sediment concentrations (BSAF) rather than as a BSAR. However, BSARs are preferred for the following reasons:

- BSAFs based on a simple ratio between sediment and tissue chemical concentrations do not allow for the possibility of background contributions to tissue from non-sediment or other sources.
- BSAFs are just a special case of BSARs (i.e., linear equations with the intercept forced to equal zero), so regression modeling will produce a BSAF if justified by the data.[6]

Both BSARs and BSAFs were developed using OC-normalized sediment chemical concentrations and lipid-normalized tissue concentrations for all chemicals except metals. For metals, unadjusted dry-weight sediment chemical concentrations and wet-weight tissue chemical concentrations were used for BSAR and BSAF development.

Benthic invertebrates, sculpin, and smallmouth bass have exposure areas that are smaller than the Study Area, and so there are multiple pairs of co-located tissue and sediment chemical concentration data. These co-located datasets were statistically evaluated to determine whether tissue concentrations were statistically related to co-located sediment concentrations, and if so, how to model that statistical relationship sediment (Section 4.1).

Black crappie, brown bullhead, peamouth, largescale sucker, northern pikeminnow, and carp range across the entire Study Area, and so these species lack multiple pairs of co-located sediment and tissue chemical concentration data. For these species, it was not possible to statistically analyze whether Study Area tissue concentrations were correlated with sediment (because there was only one sediment exposure concentration–the Study

[5] Co-located tissue and exposure areas are described for each species in Section 3.3.

[6] In cases where the data support a zero-intercept, the averaging approach (Burkhard 2006) may be used instead of the zero-intercept regression model to set the BSAF. The choice between the averaging model and regression model should take into account an analysis of the two models' residuals.

Area-wide SWAC). BSAFs were developed based on ratios of sediment and tissue chemical concentrations, as appropriate (Section 4.2).

4.1 GENERAL APPROACH FOR BSARS FOR SPECIES WITH HOME RANGES SMALLER THAN THE SITE

BSARs were developed for several preliminary COCs (see Tables 2-1 and 2-2) for those species with exposure areas smaller than the site. These species include benthic invertebrates (laboratory worms, field clams, and crayfish), sculpin, and smallmouth bass.

4.1.1 Model Development and Screening

In the first step of the BSAR development, three possible linear tissue-sediment models were developed and screened. Several potential BSARs were calculated for each receptor-preliminary COC dataset with a minimum of three co-located empirical data values. Only linear models were considered in this BSAR development process because data were rarely adequate to consider more complex models. The following linear regressions were considered for each receptor-preliminary COC dataset:

1. Untransformed tissue concentrations vs. sediment concentrations
2. Untransformed tissue concentrations vs. log-transformed sediment concentrations
3. Log-transformed tissue concentrations vs. log-transformed sediment concentrations

The strength of the tissue-sediment relationship was rated as one of the following categories based on the coefficient of determination (r^2):

- No relationship: where $0.0 \le r^2 < 0.3$
- Weak relationship: where $0.3 \le r^2 < 0.5$
- Moderate relationship: where $0.5 \le r^2 < 0.7$
- Strong relationship: where $0.7 \le r^2 < 1.0$

A regression model was accepted as a candidate BSAR if the slope was significantly different from zero ($p < 0.05$) and the r^2 was greater than 0.30 (i.e., at the minimum, a weak relationship was established).

All BSAR calculations, statistical analyses (significance levels, outlier diagnostics, and goodness-of-fit statistics), and graphical summaries were conducted in the software program R. Statistical summaries were downloaded to a Microsoft Excel® workbook, where screening steps were performed through a series of “if-then” statements. Graphical summaries and outlier diagnostic statistics were considered in the second step of the BSAR development process, the model selection step. Three samples were sufficient to attempt to develop a regression relationship; however, there were generally at least eight data pairs in the regression relationships accepted as candidate BSARs (based on strength of correlation and significance).

4.1.2 Model Selection

A BSAR was selected from the candidate models for each receptor-chemical combination. If a receptor-chemical combination had more than one candidate BSAR, visual and quantitative analyses were used to select the best model. Visual analysis involved comparison of scatter plots of tissue concentrations (y-axis) vs. sediment concentrations (x-axis) and plots of model residual distributions[7] for each of the three model types. In addition, outlier statistics, including Leverage and Cook's Distance, were calculated for each data value, and the number of potential "outliers" was identified for each model. Graphical analyses and outlier statistics were used in combination to evaluate the extent to which linearity of the tissue-sediment relationship and the variance of residuals were consistent across the range of sampled sediment concentrations and to compare the distributions of residuals around the model for each of the models that passed the initial screen.

Final BSARs were selected from the candidate models based on the following considerations:

- Consistency of linear relationship across the range of sediment concentrations
- Distribution (homogeneity of variance and normality) of residuals around model predictions
- Outlier and influence diagnostics such as Studentized residuals; leverage; slope, intercept, fit influence measures; Cook's distance
- The number and spatial distribution of influential data values (potential outliers)
- Possibility that influential or non-fitting data points indicate existence of separate or subpopulations
- Consistency of model type selected within a chemical class (e.g., selected all log-log models for PAHs because overwhelming majority of best performing models for PAHs were log-log models)
- Logical consistency of predictions of bioaccumulation (e.g., significant intercept greater than zero indicating significant background water or prey exposure; negative intercept possibly indicating bioregulation)

Tables 4-1 to 4-5 present the best-fit models chosen from the BSAR candidates for all receptor-chemical combinations where BSARs were appropriate. If no model fit a dataset, indicating that tissue residues were unrelated to sediment chemical concentrations, no BSAR was selected. The lack of a relationship between sediment and tissue concentrations might indicate water column mixing and the transport of chemicals released from sediment,

[7] Plots of model residual distributions included plots of ordered residual values, q-q plots of residuals, and scatter plots of residuals vs. predicted values and residuals vs. leverage values.

that a medium other than sediment is the source of the tissue residue (e.g., upstream or lateral loads to surface water), that organisms are bioregulating (particularly relevant in the case of essential metals) or metabolizing the chemical (e.g., fish metabolize PAHs), or that the exposure area or use of the exposure area by organisms was not described well enough to define a relationship. All of the selected BSARs were based on log-log transformations of the sediment and tissue data. The log-log transformations were necessary to obtain reasonable spread on the independent variables in the regression analyses and improve model fit.

Table 4-1. Selected BSARs for Field Clams

Chemical	Selected BSAR[a]	Model Type	Correction Factor[b]	r^2
Metals				
Arsenic	No relationship[c]	NA	NA	NA
Cadmium	No relationship[c]	NA	NA	NA
Copper	No relationship[c]	NA	NA	NA
Zinc	No relationship[c]	NA	NA	NA
PAHs				
Benzo(a)anthracene	$\ln(C_{tiss}) = 0.588 \times \ln(C_{sed}) + \ln(CF) - 0.97$	log-log	1.70	0.40
Benzo(a)pyrene	$\ln(C_{tiss}) = 0.60 \times \ln(C_{sed}) + \ln(CF) - 2.47$	log-log	2.31	0.36
Benzo(b)fluoranthene	No relationship[c]	NA	NA	NA
Benzo(k)fluoranthene	$\ln(C_{tiss}) = 0.707 \times \ln(C_{sed}) + \ln(CF) - 2.55$	log-log	2.13	0.43
Chrysene	$\ln(C_{tiss}) = 0.486 \times \ln(C_{sed}) + \ln(CF) - 0.66$	log-log	1.57	0.34
Dibenzo(a,h)anthracene	No relationship[c]	NA	NA	NA
Indeno(1,2,3-cd)pyrene	No relationship[c]	NA	NA	NA
Phthalates				
BEHP	Insufficient data to determine BSAR[d]	NA	NA	NA
Dibutyl phthalate	Insufficient data to determine BSAR[d]	NA	NA	NA
Butyltins				
Tributyltin	No relationship[c]	NA	NA	NA
SVOCs				
Hexachlorobenzene	No relationship[c]	NA	NA	NA

[a] All BSARs based on lipid-normalized tissue and OC-normalized sediment data, with the exception of metals where BSARs are based on wet-weight tissue and dry-weight sediment data.

[b] Correction factors were used for log-log BSAR models. The use of the correction factor in calculating PRGs is explained in Section 4.4.

[c] No appropriate BSAR could be developed because the linear and log-linear models had either an $r^2 < 0.30$ or an insignificant slope.

[d] Not enough detect-detect tissue-sediment data pairs

BEHP – bis(2-ethylhexyl) phthalate

NA – not applicable

BSAR – biota-sediment accumulation regression
CF – correction factor
C_{sed} – sediment concentration
C_{tiss} – tissue concentration
OC – organic carbon
PAH – polycyclic aromatic hydrocarbon
PRG – preliminary remediation goal
SVOC – semivolatile organic compound

Table 4-2. Selected BSARs for Crayfish

Chemical	Selected BSAR[a]	Model Type	Correction Factor[b]	r^2
Metals				
Arsenic	No relationship[c]	NA	NA	NA
Copper	No relationship[c]	NA	NA	NA
Lead	No relationship[c]	NA	NA	NA
PAHs				
Benzo(a)anthracene	Insufficient data to determine BSAR[d]	NA	NA	NA
Benzo(a)pyrene	$\ln(C_{tiss}) = 0.983 \times \ln(C_{sed}) + \ln(CF) - 5.54$	log-log	1.09	0.92
Benzo(b)fluoranthene	Insufficient data to determine BSAR[d]	NA	NA	NA
Benzo(k)fluoranthene	Insufficient data to determine BSAR[d]	NA	NA	NA
Chrysene	Insufficient data to determine BSAR[d]	NA	NA	NA
Dibenzo(a,h)anthracene	Insufficient data to determine BSAR[d]	NA	NA	NA
Indeno(1,2,3-cd)pyrene	Insufficient data to determine BSAR[d]	NA	NA	NA
Butyltins				
Tributyltin	No relationship[c]	NA	NA	NA
SVOCs				
Hexachlorobenzene	No relationship[c]	NA	NA	NA
Pentachlorophenol	Insufficient data to determine BSAR[d]	NA	NA	NA

[a] All BSARs based on lipid normalized tissue and OC-normalized sediment data, with the exception of metals where BSARs are based on wet weight tissue and dry weight sediment data.

[b] Correction factors were used for log-log BSAR models. The use of the correction factor in calculating PRGs is explained in Section 4.4.

[c] No appropriate BSAR could be developed because the linear and log linear models had either an $r^2 < 0.30$ or an insignificant slope.

[d] Not enough detect-detect tissue sediment data pairs

BEHP – bis(2-ethylhexyl) phthalate
BSAR – biota-sediment accumulation regression
CF – correction factor
C_{sed} – sediment concentrations
C_{tiss} – tissue concentration
NA – not applicable
OC – organic carbon
PAH – polycyclic aromatic hydrocarbon
PRG – preliminary remediation goal
SVOC – semivolatile organic compound

Table 4-3. Selected BSARs for Laboratory Worms

Chemical	Selected BSAR[a]	Model Type	Correction Factor[b]	r^2
Metals				
Arsenic	No relationship[c]	NA	NA	NA
Cadmium	No relationship[c]	NA	NA	NA
Copper	No relationship[c]	NA	NA	NA
Zinc	No relationship[c]	NA	NA	NA
PAHs				
Benzo(a)pyrene	$\ln(C_{tiss}) = 0.618 \times \ln(C_{sed}) + \ln(CF) - 0.48$	log-log	1.83	0.393
Butyltins				
Tributyltin	$\ln(C_{tiss}) = 0.968 \times \ln(C_{sed}) + \ln(CF) - 1.67$	log-log	1.52	0.66

[a] All BSARs based on lipid normalized tissue and OC-normalized sediment data, with the exception of metals where BSARs are based on wet weight tissue and dry weight sediment data.

[b] Correction factors were used for log-log BSAR models. The use of the correction factor in calculating PRGs is explained in Section 4.4.

[c] No appropriate BSAR could be developed because the linear and log linear models had either an $r^2 < 0.30$ or an insignificant slope.

BSAR – biota-sediment accumulation regression
CF – correction factor
C_{sed} – sediment concentrations
C_{tiss} – tissue concentration
NA – not applicable
OC – organic carbon
PAH – polycyclic aromatic hydrocarbon
PRG – preliminary remediation goal

Table 4-4. Selected BSARs for Sculpin

Chemical	Selected BSAR[a]	Model Type	Correction Factor[b]	r^2
Metals				
Cadmium	No relationship[c]	NA	NA	NA
Copper	No relationship[c]	NA	NA	
Lead	$\ln(C_{tiss}) = 0.610 \times \ln(C_{sed}) + \ln(CF) - 0.486$	log-log	1.29	0.486
Butyltins				
Tributyltin	No relationship[c]	NA	NA	NA

[a] All BSARs based on lipid normalized tissue and OC-normalized sediment data, with the exception of metals where BSARs are based on wet weight tissue and dry weight sediment data.

[b] Correction factors were used for log-log BSAR models. The use of the correction factor in calculating PRGs is explained in Section 4.4.

[c] No appropriate BSAR could be developed because the linear and log linear models had either an $r^2 < 0.30$ or an insignificant slope.

BSAR – biota-sediment accumulation regression
CF – correction factor
C_{sed} – sediment concentration
C_{tiss} – tissue concentration
NA – not applicable
OC – organic carbon
PRG – preliminary remediation goal

Table 4-5. Selected BSARs for Smallmouth Bass

Chemical	Selected BSAR[a]	Model Type	Correction Factor[b]	r^2
Metals				
Antimony	No relationship[c]	NA	NA	NA
Arsenic	No relationship[c]	NA	NA	NA
Lead	No relationship[c]	NA	NA	NA
Mercury	No relationship[c]	NA	NA	NA
Selenium	No relationship[c]	NA	NA	NA
Zinc	No relationship[c]	NA	NA	NA
PAHs				
Benzo(a)anthracene	No relationship[c]	NA	NA	NA
Benzo(a)pyrene	No relationship[c]	NA	NA	NA
Dibenzo(a,h)anthracene	Insufficient data to determine BSAR[d]	NA	NA	NA
Phthalates				
BEHP	No relationship[c]	NA	NA	NA
SVOCs				
Hexachlorobenzene	No relationship[c]	NA	NA	NA

a All BSARs based on lipid normalized tissue and OC-normalized sediment data, with the exception of metals where BSARs are based on wet weight tissue and dry weight sediment data.

b Correction factors were used for log-log BSAR models. The use of the correction factor in calculating PRGs is explained in Section 4.4.

c No appropriate BSAR could be developed because the linear and log linear models had either an $r^2 < 0.30$ or an insignificant slope.

d Not enough detect-detect tissue sediment data pairs

BEHP – bis(2-ethylhexyl) phthalate
BSAR – biota-sediment accumulation regression
CF – correction factor
C_{sed} – sediment concentrations
C_{tiss} – tissue concentration
NA – not applicable
OC – organic carbon
PAH – polycyclic aromatic hydrocarbon
PRG – preliminary remediation goal
SVOC – semivolatile organic compound

4.2 LARGE-HOME-RANGE SPECIES BSAFS

BSAFs were developed for black crappie, northern pikeminnow, peamouth, carp, largescale sucker, and brown bullhead. BSAFs are the ratio of Study Area-wide tissue to sediment chemical concentrations. The tissue concentration was the average of available composite samples for each species, and the sediment concentration was the Study Area SWAC based on a natural neighbor interpolation.[8] If at least one BSAR for a smaller-home-range species (Section 4.1.2) could be identified for a given chemical, then a BSAF was developed for that chemical. However, if no BSARs were identified for a chemical (due to a lack of data or inability to reasonably describe a tissue-sediment relationship, see Tables 4-1 through 4-5), then no BSAFs for large-home-range species were calculated for that chemical, to prevent BSAFs from being used inappropriately to derive PRGs when there was no evidence that reducing sediment concentration would result in lower tissue concentrations.

BSAFs express the assumed steady-state relationship between the measured concentration of a bioaccumulating chemical in sediment and that in tissue.

BSAFs for organic preliminary COCs were derived using Equation 4-1:

$$\mathrm{BSAF} = \frac{(C_{\mathrm{tiss,LN}})}{(C_{\mathrm{sed,OC}})} \qquad \textbf{Equation 4-1}$$

Where:

$BSAF$ = site-specific fish BSAF
$C_{tiss,LN}$ = fish tissue concentration, lipid-normalized (mg/kg lipid dw)
$C_{sed,OC}$ = surface sediment concentration, OC-normalized (mg/kg OC dw)

BSAFs for metals were derived using Equation 4-2:

$$\mathrm{BSAF} = \frac{(C_{\mathrm{tiss,ww}})}{(C_{\mathrm{sed,dw}})} \qquad \textbf{Equation 4-2}$$

Where:

$BSAF$ = site-specific fish BSAF
$C_{tiss,ww}$ = fish tissue concentration (mg/kg ww)
$C_{sed,dw}$ = surface sediment concentration (mg/kg dw)

Table 4-6 presents the BSAFs for black crappie, brown bullhead, peamouth, northern pikeminnow, sucker, and carp.

[8] It is worth noting that natural neighbors interpolation and the Thiessen polygon method yields identical study area SWACs (de Smith et al. 2008). Thiessen polygons were used previously to derive SWACs specified in the *Comprehensive Round 2 Site Characterization Summary and Data Gaps Analysis Report* (Integral et al. 2007).

Table 4-6. BSAFs for Large-Home-Range Species

		BSAF Equation[b]						
Chemical	**BSAF Use[a]**	**Black Crappie**	**Brown Bullhead**	**Carp**	**Lamprey**	**Largescale Sucker**	**Northern Pikeminnow**	**Peamouth**
Metals								
Antimony	Yes[c]	$C_t = 0.000802 \times C_s$	$C_t = 0.000802 \times C_s$	$C_t = 0.00353 \times C_s$				
Arsenic	No	NM	NM	NM				
Copper	No				NM	NM		
Lead	Yes	$C_t = 0.000269 \times C_s$	$C_t = 0.00102 \times C_s$	$C_t = 0.00817 \times C_s$		$C_t = 0.00490 \times C_s$	$C_t = 0.000359 \times C_s$	$C_t = 0.110 \times C_s$
Mercury	No	NM	NM	NM		NM	NM	NM
Selenium	No	NM	NM	NM				
Zinc	No	NM	NM	NM				
PAHs								
Benzo(a)anthracene	Yes	NTD	$C_t = 0.0139 \times C_s$	$C_t = 0.00168 \times C_s$				
Benzo(a)pyrene	Yes	NTD	$C_t = 0.0109 \times C_s$	$C_t = 0.00132 \times C_s$				
Dibenzo(a,h)anthracene	Yes[c]	NTD	$C_t = 0.107 \times C_s$	$C_t = 0.0129 \times C_s$				
Phthalates								
BEHP	No	NM	NM	NM				
Butyltins								
Tributyltin	Yes			$C_t = 0.00499 \times C_s$				
SVOCs								
Hexachlorobenzene	Yes[c]	$C_t = 0.295 \times C_s$	$C_t = 2.02 \times C_s$	$C_t = 0.244 \times C_s$				

[a] BSAFs were not used if no BSAR could be developed for any small-home range-species (laboratory clams, field clams, laboratory worms, and crayfish) or medium-home-range species (sculpin and smallmouth bass).

[b] All BSAFs based on lipid-normalized tissue and OC-normalized sediment data, with the exception of metals for which BSAFs are based on wet-weight tissue and dry-weight sediment data.

[c] No BSAR for these chemicals is shown in Tables 4-1 to 4-5 because it was not needed for PRG development, but a BSAR was available for lab worms for these chemicals. Therefore BSAFs for this chemical were developed.

BEHP – bis(2-ethylhexyl) phthalate
BSAF – biota-sediment accumulation factor
C_s – chemical concentration in sediment
C_t – chemical concentration in tissue
NM – no model developed
NTD – no tissue data
OC – organic carbon
PAH – polycyclic aromatic hydrocarbon
PRG – preliminary remediation goal
SVOC – semivolatile organic compound

4.3 SUMMARY OF BSAR/F AVAILABILITY FOR DIFFERENT SPECIES

Table 4-7 presents a summary of the chemical-species combinations for which BSAFs or BSARs were developed. All of the selected BSARs were based on log-log transformations of the sediment and tissue data. The BSAFs or BSARs were used for the calculation of PRGs. BSARs could not be developed for some preliminary COCs because of insufficient data (i.e., too many non-detect tissue concentration values) or because none of the models appeared to fit the dataset across the range of sample concentrations. As noted in Section 4.2, if a BSAR for at least one species for a given chemical could not be developed, then no BSAFs for that chemical were developed.

Table 4-7. Summary of BSAF and BSAR Availability

	Small- and Medium-Home-Range Species[a]					Large-Home-Range Species[a]						
Chemical	**Field Clam**	**Crayfish**	**Lab Worm**	**Sculpin**	**Smallmouth Bass**	**Black Crappie**	**Brown Bullhead**	**Carp**	**Lamprey**	**Largescale Sucker**	**Northern Pikeminnow**	**Peamouth**
Metals												
Antimony					N – NM	Y[b]	Y[b]	Y[b]				
Arsenic	N – NM	N – NM	N – NM		N – NM	N – NA	N – NA	N – NA				
Cadmium	N – NM		N – NM	N – NM								
Copper	N – NM	N – NM	N – NM	N – NM					N – NA	N – NA		
Lead		N – NM		Y	N – NM	Y	Y	Y		Y	Y	Y
Mercury					N – NM	N – NA	N – NA	N – NA		N – NA	N – NA	N – NA
Selenium					N – NM	N – NA	N – NA	N – NA				
Zinc	N – NM		N – NM		N – NM	N – NA	N – NA	N – NA				
PAHs												
Benzo(a)anthracene	Y	N – ISD			N – NM	N – NTD	Y	Y				
Benzo(a)pyrene	Y	Y	Y		N – NM	N – NTD	Y	Y				
Benzo(b)fluoranthene	N – NM	N – ISD										
Benzo(k)fluoranthene	Y	N – ISD										
Chrysene	Y	N – ISD										
Dibenzo(a,h)anthracene	N – NM	N – ISD			N – ISD	N – NTD	Y[b]	Y[b]				
Indeno(1,2,3-cd)pyrene	N – NM	N – ISD										
Phthalates												
BEHP	N – ISD				N – NM	N – NA	N – NA	N – NA				
Dibutyl phthalate	N – ISD											
SVOCs												
Hexachlorobenzene	N – NM	N – NM			N – NM	Y[b]	Y[b]	Y[b]				

Table 4-7. Summary of BSAF and BSAR Availability

	Small- and Medium-Home-Range Species[a]					Large-Home-Range Species[a]						
Chemical	**Field Clam**	**Crayfish**	**Lab Worm**	**Sculpin**	**Smallmouth Bass**	**Black Crappie**	**Brown Bullhead**	**Carp**	**Lamprey**	**Largescale Sucker**	**Northern Pikeminnow**	**Peamouth**
Pentachlorophenol		N – ISD										
Butyltins												
Tributyltin	N – NM	N – NM	Y	N – NM				Y				

[a] The availability of BSAR or BSAF models is indicated by a "Y" (model available) or an "N" (no model available). Blanks indicate that the model was not needed for PRG development. Reasons for unavailable BSAR models include the following:

ISD – insufficient data to develop a BSAR (i.e., not enough detect-detect tissue sediment data pairs)

NA – BSAF not applicable because BSAR models could not be developed for small- or medium-home-range species

NC – model for TEQ conversion did not pass screening requirements (significant slope and $r^2 > 0.3$)

NM – no model developed; no BSAR model passed screening requirements (significant slope and $r^2 > 0.3$)

NTD – tissue not analyzed for this chemical, and thus no BSAF could be developed

[b] No BSAR for these chemicals is shown for a small- or medium-home-range species because it was not needed for PRG development. However, a BSAR was available for laboratory worms for these chemicals, and thus BSAFs were developed for large-home-range species as needed.

BEHP – bis(2-ethylhexyl) phthalate
BSAF – biota-sediment accumulation factor
BSAR – biota-sediment accumulation regression
N – no
PAH – polycyclic aromatic hydrocarbon
PRG – preliminary remediation goal
SVOC – semivolatile organic compound
TEQ – toxic equivalent
Y – yes

4.4 PRG DEVELOPMENT USING BSARS AND BSAFS

The calculation of PRGs involved several steps. If the PRG was based on a tissue line of evidence for an ecological receptor, then BSAR/Fs were used to estimate the sediment concentration associated with the TRV tissue concentration. If the PRG was based on a dietary line of evidence (as with diet-based ecological PRGs or the human health PRGs which were based on fish or shellfish consumption), then the sediment concentration associated with the target prey or diet tissue concentration was estimated. Because some diets consist of multiple species, sometimes a range of PRGs was generated to reflect exclusive consumption of the most and least bioaccumulating species that could be modeled. In some cases, BSARs could not be developed for all species consumed because data for BSAR development were insufficient or because no relationship was found.

When using BSARs to estimate sediment PRGs, it was necessary to apply a correction factor because the BSARs were based on linear relationships for log-log transformations of sediment and tissue data. BSAR equations were developed with the independent variable (Y) equal to the tissue concentration~~,~~ and the dependent variable (X) equal to the sediment concentration, as shown in Equation 4-3. ~~The application of the correction factors for estimation of PRGs is explained in Appendix C.~~

$$X = EXP\left(\frac{\ln(Y) - \ln(F) - a}{b}\right)$$

Equation 4-3

Where:

Y = independent variable
X = dependent variable
a = model intercept
b = model slope
F = correction factor

Field Code Changed

Early PRGs using BSARs were developed and presented in the Early PRG report (Windward et al. 2009)

4.5 BSAR/F UNCERTAINTIES

A major uncertainty with BSAR/Fs is the uncertainty about appropriate exposure areas. Literature reviews were performed to make best estimates of such areas, but there is significant uncertainty regarding the movements and habitat use by both the species modeled and their prey.

There is no significance test for BSAFs (which are simply average concentration ratios). With BSARs the statistical significance of the relationship and confidence interval for the slope and intercept as well as predictions can be quantified. With BSAFs, the relationship may be based on only a few detected concentrations. Hence, the BSAF modeling approach has the greatest uncertainty (compared to BSARs or mechanistic modeling).

For the majority of chemical-species combinations for which BSARs were attempted, few BSARs could be developed either because data were insufficient or no model passed the screen (Table 4-7). In cases when a BSAR could be developed, the relationship was usually weak (i.e., r^2= 0.3 to 0.5).

For field clams, only four BSARs were developed, all with weak relationships; and no relationship was identified for 9 of the 16 chemicals assessed. For the remaining chemicals, data were insufficient to attempt BSAR development. For crayfish, there were insufficient data for most chemicals primarily because of a large number of non-detected~~ND~~ tissue data. Only one BSAR model passed for crayfish: benzo(a)pyrene. This relationship was "strong" (r^2=0.92), but it was driven by a single, high-leverage, high-concentration data point. For laboratory worms, only two BSARs were developed (of six attempted) and of those, one chemical had only a weak relationship (benzo[a]pyrene). TBT had a moderate relationship (r^2 = 0.66) for worms, but this was driven largely by a single data point with high leverage. Only one model was developed for sculpin (lead), and this model had only a weak relationship. No models could be developed for any of the chemicals evaluated for BSARs for smallmouth bass.

As previously mentioned, because BSAFs are simply a ratio of Study Area-wide average tissue and sediment concentrations, they cannot be evaluated for statistical significance or strength of relationship. Therefore, the BSARs for a chemical were used to evaluate whether tissue-sediment relationships exist for that chemical, and if no BSAR could be developed, BSAFs were not developed. In the absence of a BSAR relationship, there is no logical basis for using BSAFs to derive PRGs.

4.6 UNCERTAINTIES ASSOCIATED WITH APPLICATION OF BSAF/RS FOR PRG DEVELOPMENT

When estimating early PRGs for consumers of multi-species diets, a range of early PRGs was generated because of the difficulty of calculating a PRG based on a multi-species diet, given that different regression relationships (i.e. BSARs or BSAFs) were developed for each species. If a PRG for each apportioned dietary scenario were calculated, it would fall within the range of the early PRGs estimates.

BSARs lack power to predict beyond the range of the data used to build the model, or to predict when the conditions underlying the data used to build the model change. PRGs derived from BSARs can be no better than the models used to generate them (e.g., if only a weak relationship was found between sediment and tissue, there should be less confidence in the resulting PRG than if a strong relationship was found). BSARs and BSAFs also do not explicitly account for water contribution to exposure. If there were a background contribution from water (e.g., entering Portland Harbor from upstream), BSAFs would not differentiate the water's contribution to chemical contamination in tissue from that of sediments or any other source. BSARs would be able to account for current background contributions (they would be reflected in a positive y-intercept), but only mechanistic modeling can account for changes in background contribution under different conditions (e.g., if sediment SWACs were reduced). Because of these limitations, BSAR/Fs are strictly appropriate only for estimating tissue concentrations under current conditions (e.g., filling gaps in baseline risk assessment datasets). In the absence of a mechanistic model, a statistical model (BSAR/F) might be used to derive PRGs.

5.0 MECHANISTIC MODEL

As discussed previously, the mechanistic model is appropriate for modeling some hydrophobic organic chemicals (Arnot and Gobas 2004) and was applied for many of the chemical-species combinations for which PRGs were desired (Tables 2-1 and 2-2), including PCBs, the chemicals responsible for most of the potential human health and ecological risk.

5.1 MODELING GOALS AND APPLICATIONS

The overall goal of the mechanistic modeling described in this report for the Portland Harbor RI/FS was to develop predictive relationships between chemical concentrations in sediment, water, and tissue, both now and under a variety of prospective remedial action scenarios. Specifically, the goal was to use the mechanistic model to derive PRGs for hydrophobic organic compounds (e.g., PCBs, DDTs, and dioxin-like compounds).

Section 5.2 briefly compares the Round 2 Report (Integral et al. 2007) model to the updated model and Section 5.3 presents the processes for model development and calibration. Sections 5.4 through 5.6 present model performance results, model sensitivity analysis, and uncertainty analysis for the model and PRGs, respectively. The PRGs calculated using the mechanistic model were presented in the Early PRG Report (Windward et al. 2009).

5.2 COMPARISON TO ROUND 2 REPORT MODEL

As compared to the model developed as part of the Round 2 Report (Integral et al. 2007), the updated model presented here has numerous modifications. The basic model structure and assumptions have not changed. However, some improvements in the parameterization and calibration have been made and are summarized here.

The first important difference from the Round 2 Report model was the significantly larger dataset. Sediment, water, and tissue data were collected as part of the Round 3 sampling efforts, which allowed for improved parameterization and calibration of the model. Improved detection limits in the Round 3 dataset improved model performance for DDT compounds, and the additional Round 3 data made it possible to use the mechanistic model for all the pesticide COCs.

Second, the distributions for several key parameters were improved as follows:

- Chemical-specific octanol-water partition coefficient (K_{OW}) – To be consistent with the values used in the RI, a larger set of literature sources was used to determine the K_{OW}. Additionally, uniform distributions were used to better capture the uncertainty surrounding this parameter (see Section 5.3.5.2.3 and Appendix ~~D~~ B for additional information).
- Chemical concentration in water – Additional water data were collected as part of the Round 3 sampling effort, which greatly increased the breadth and complexity of

the dataset (variability in location, season, flow rate, etc.). An averaging scheme was used to better characterize the Study Area-wide chemical concentrations in water, as discussed in Appendix ~~D~~B.

- Metabolic rate constant (K_M) – For chemicals known to be metabolized, additional research was done regarding the ~~metabolic rate constant~~K_Ms to better account for this process in the model (see Section 5.3.5.2.4 and Appendix ~~D~~ B for additional information).
- Dietary distributions – Uniform distributions (as opposed to triangular distributions used in the Round 2 Report model) were used for the diets of modeled species. With the exception of sculpin, the dietary compositions were not altered. The diet of sculpin was refined to better represent the size class of sculpin being modeled and consumed by species in higher trophic levels (see Appendix ~~D~~B).

The improved distributions used for these parameters allowed for enhanced model calibration.

A third important difference from the Round 2 Report model was the altered calibration process (see Section 5.3.5.3). Instead of using an individual PCB congener for the initial model calibration, total PCBs was used both because it had a larger dataset and because it had been identified as a major contributor to risk in both the BERA (Windward 2013) and the BHHRA (Kennedy/Jenks 2013). In addition, rather than focusing on the average model performance, the model's predictive ability for smallmouth bass was prioritized because of the importance of this species for PRG development and ultimately remediation decisions. Thus, model performance was based first on bass, while also attempting to optimize model performance for other species. In addition, the model calibration was verified on a smaller spatial scale (for smallmouth bass) early in the calibration process to ensure that the model was able to predict both on a Study Area--wide basis and for individual exposure areas.

As a result of these changes, performance for the model was improved as compared to the Round 2 Report model. A full discussion of the results is presented in Section 5.4.

5.3 MODEL DEVELOPMENT AND METHODOLOGY

The Arnot and Gobas model (Arnot and Gobas 2004; EPA 2006) was selected after an evaluation of several different mechanistic bioaccumulation models (Windward 2005, 2004), was used to develop initial PRGs (iPRGs) in the Comprehensive Round 2 Report (Integral et al. 2007), and was used here to develop PRGs. The Arnot and Gobas model (2004) includes several advances over previous Gobas-type models; these were discussed in the 2005 bioaccumulation modeling report (Windward 2005). This model is most appropriate for hydrophobic organic chemicals. Some general underlying assumptions include:

- The aquatic system is in steady state with respect to bioaccumulation of hydrophobic organic chemicals.

- The flux of chemicals between water and organisms, between ingested media (i.e., sediment and other organisms) and organism tissue, and between different tissue types (e.g., lipid and non-lipid organic matter) are governed by fugacity relationships (Arnot and Gobas 2004).

The above assumptions are generally made for applications of Gobas-type models, which have been used for a variety of sites including rivers, lakes, and estuaries. The model structure and additional model assumptions are discussed in the following subsections.

5.3.1 Species to be Modeled

The use of an overly detailed mechanistic model with numerous species categories would have exceeded both the availability of site-specific and literature-derived physiological data (ODEQ 2006). The Lower Willamette River food web modeling working group, which consists of LWG members and EPA and its partners, had several discussions to agree on the species to be modeled. EPA and its partners stated, "as the model's primary purpose is to inform remediation decisions and not to precisely predict tissue residues, a simplified food web, encompassing pelagic and benthic species, should be sufficient at this time" (EPA 2006). Based on this premise, certain representative pelagic and benthic species were selected for modeling through negotiations within the Lower Willamette River FWM working group. The trophic groups modeled, and the representative species for which LWG data are available (listed in parentheses), are the same as those used for modeling presented in the Round 2 Report (Integral et al. 2007) and are as follows:

- Phytoplankton
- Zooplankton
- Benthic infaunal invertebrate filter feeders (BIF) (clams, *Corbicula fluminea*)
- Benthic infaunal invertebrate consumers (BIC)[9]
- Epibenthic invertebrate consumers (EICs) (crayfish [note that crayfish samples were not identified by species])
- Foraging fish (sculpin, *Cottus* sp.)[10]
- Benthivorous fish (largescale sucker, *Catostomus macrocheilus*)[11]
- Omnivorous fish (common carp, *Cyprinus carpio*)
- Small piscivorous fish (smallmouth bass, *Micropterus dolomieui*)
- Large piscivorous fish (northern pikeminnow, *Ptychocheilus oregonensis*)

[9] A generalized category designed to represent oligochaetes, insect larvae, and amphipods.

[10] This trophic group was also used to represent black crappie and peamouth for PRG development.

[11] This trophic group was also used to represent brown bullhead for PRG development.

5.3.2 Development of Visual Basic for Applications® Model

The LWG was provided with a Visual Basic for Applications® (VBA) version of the Arnot and Gobas (2004) model by Dr. Bruce Hope, a senior environmental toxicologist with ODEQ (ODEQ 2006). In this version of the model, an Excel® workbook uses imbedded VBA macros to perform calculations. This version of the model was evaluated and adjusted in collaboration with Dr. Hope to ensure that it functioned in the same manner as the original Arnot and Gobas version of the model, and was used to calculate iPRGs in the Comprehensive Round 2 Report. The equations used in the modified model and general model assumptions are the same as those in the Arnot and Gobas model (2004). These equations along with the actual VBA code are described in a detail in Appendix ~~E~~C.

5.3.3 Selection of Chemicals to be Modeled

The mechanistic model was applied to several hydrophobic organic chemicals, including PCBs, dioxins, and pesticides (see Tables 2-1 and 2-2). The following subsections describe the chemicals that were used to calibrate the model and the chemicals to which the model was applied for PRG development.

5.3.3.1 Chemicals Used for Initial Model Calibration

Numerous parameters in the mechanistic model are not chemical-specific (e.g., lipid content of zooplankton). Accurate values for parameters common to all chemicals (hereafter referred to as non-chemical-specific parameters) must be selected so that the model can perform well for a range of chemicals. Four individual chemicals and two chemical groups were selected for the development of optimal values for non-chemical-specific input parameters. The non-chemical-specific parameters that were calibrated in this step include the following:

- General environmental parameters: water temperature, total suspended solids in water, dissolved OC concentration in water, and OC content of sediment

- Species-specific biological and dietary parameters: weight, lipid content, moisture content, fraction of porewater ventilated, growth rate constant, and dietary consumption fractions

For model calibration, it was desirable to have chemicals with a range of K_{OW} values. Total PCBs was selected as the initial calibration chemical because of its importance for establishing PRGs for the Portland Harbor Study Area. Additionally, the large dataset for total PCBs helped ensure that the total PCBs model would be most accurately calibrated. To the extent that this improved the calibration of non-chemical-specific parameters, it also improved the calibration for other chemicals. Five additional chemicals with K_{ow} values ranging from 5.70 to 7.48 were then used to verify the model (i.e., confirm that the model was able to predict tissue concentration for chemicals with different properties). These chemicals included 4,4′-DDE, total DDx, PCB 17, PCB 118, and PCB 167. The selection of both individual chemicals (4,4′-DDE and the PCB congeners) and chemical mixtures (total

PCBs and total DDx) helped to ensure that the model would be calibrated to perform well for a variety of chemicals. Several criteria were used to select the calibration chemicals:

- First, chemicals for calibration that represented a range of K_{OW} values were chosen so that model performance could be evaluated across the spectrum of K_{OW} values. It was important to select chemicals that had a range of K_{OW}s because the model is highly sensitive to $K_{OW,}$ which is involved in numerous model equations (see Appendix ~~E~~C) (Arnot and Gobas 2004).
- Second, chemicals with a high frequency of detection in sediment, water, and tissue were chosen. Appendix ~~D~~ B provides details on the frequency of detection and the concentrations of these chemicals in water, sediment, and tissue samples.
- Third, PCB congeners that did not co-elute during chemical analysis were chosen because co-elution makes it difficult to interpret concentration data.
- Fourth, chemicals that were not significantly metabolized were selected to minimize the impact of uncertain metabolic rates on model calibration.

Model performance metrics are described in Section 5.3.4, and model calibration is described in detail in Section 5.3.5.

5.3.3.2 Chemicals and Chemical Groups for PRG Development

After initial model calibration (for non-chemical-specific parameters), the chemical-specific parameters of the model were calibrated for each chemical for which PRGs were needed. These included PCBs, dioxins/furans, and pesticides (Table 5-1). ~~For TEQ mixtures a surrogate was used for development of PRGs. The selection of surrogates was described in Section 3.2.~~

Table 5-1. COCs for which a Calibrated Model was Developed

Chemical Group	Chemicals Modeled~~Surrogate~~
PCBs	Total PCBs[a] PCB 77 PCB 126
~~Total PCBs[a]~~	~~NA~~
~~PCB TEQ (birds)~~	~~PCB 77~~
~~PCB TEQ (mammals)~~	~~PCB 126~~
Dioxins (see Section 6)	1,2,3,7,8-PentaCDD 2,3,7,8-TetraCDD
~~Dioxins and~~ Furans (see Section 6)	1,2,3,4,7,8-HexaCDF 2,3,4,7,8-PentaCDF 2,3,7,8-TetraCDF
~~Dioxin/furan TEQ (birds)~~	~~2,3,4,7,8-PeCDF~~
~~Dioxin/furan TEQ (mammals)~~	~~2,3,4,7,8-PeCDF~~

Table 5-1. COCs for which a Calibrated Model was Developed

Chemical Group	Chemicals Modeled~~Surrogate~~	
Pesticides	Aldrin Total chlordane Sum DDD Sum DDE Sum DDT Total DDx	Dieldrin alpha-HCH beta-HCH gamma-HCH Heptachlor Heptachlor epoxide
~~Aldrin~~	~~NA~~	
~~Total chlordane~~	~~NA~~	
~~Sum DDD~~	~~NA~~	
~~Sum DDE~~	~~NA~~	
~~Sum DDT~~	~~NA~~	
~~Total DDx~~	~~NA~~	
~~Dieldrin~~	~~NA~~	
~~alpha-HCH~~	~~NA~~	
~~beta-HCH~~	~~NA~~	
~~gamma-HCH~~	~~NA~~	
~~Heptachlor~~	~~NA~~	
~~Heptachlor epoxide~~	~~NA~~	

[a] Total PCBs were calculated as the sum of congeners, when available. When congener data were not available, the sum of Aroclors was used.

CDD – chlorodibenzo-*p*-dioxin
CDF – chlorodibenzofuran
COC – chemical of concern
DDD – dichlorodiphenyldichloroethane
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
HCH – hexa~~o~~chlorocyclohexane
NA – not applicable (no surrogate needed)
PCB – polychlorinated biphenyl
~~PeCDF – pentachlorodibenzofuran~~
~~TEQ – toxicity equivalent~~
total DDx – sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE and 4,4′-DDT)

For the purpose of this report, chemical-specific parameters refer to those parameters used for the modeling of a specific chemical. Some of these parameters, such as chemical concentration in water and sediment are also site-specific parameters. K_{OW}, chemical concentration in water, and K_M~~metabolic rate constant~~s (when appropriate) were calibrated for each chemical for a specific sediment concentration. Details on the calibration and PRG development process are presented in Section 5.3.5.

5.3.4 Model Performance Metrics

One model performance metric was used to characterize the ability of the model to predict tissue chemical concentrations at specified sediment and water chemical concentrations. The primary model evaluation metric used was the species predictive accuracy factor (SPAF). The SPAF can be calculated in one of two ways: 1) if the model is over-predicting, such that the predicted value is greater than the empirical value, then the SPAF is calculated by dividing the predicted value by the empirical value, or 2) if the model is under-predicting, the SPAF is calculated by dividing the empirical value by the predicted value. Thus the SPAF is always a positive value greater than 1 (Equation 5-1).

SPAF = predicted/empirical or SPAF = empirical/predicted **Equation 5-1**

The Lower Willamette River FWM working group established a performance goal of predictive capability within a factor of 10 (average of all modeled groups). For the purpose of this report, a factor of 10 (average of all trophic groups) was considered the minimum model performance and an average factor of 3 was identified as a target. By definition, a SPAF of 1 demonstrates that the model is exactly predicting the empirical data.

5.3.5 Modeling Approach

Model calibration was performed through probabilistic analysis. An overview of the calibration process is presented here, and details are presented in Section 5.3.5.2. Briefly, the model for total PCBs was selected for initial calibration (Section 5.3.3.1), and was run 50,000 times using Monte Carlo simulation (performed using Crystal Ball® software) with different combinations of plausible values for all calibrated, non-chemical-specific model input parameters.[12] The best performing model run (i.e., the one with the lowest SPAF, especially for smallmouth bass and a realistic set of ~~mean temperature~~ parameter values ~~similar to empirical data~~) was identified. Model predictions of smallmouth bass tissue concentrations were emphasized in the calibration process because this species is particularly important for PRG development. Smallmouth bass were associated with higher risks (as a consumed species) than many other species; and because their home range is smaller than the Study Area, bass may be important in determining smaller-scale (smaller than Study Area-wide) AOPCs. The values for non-chemical-specific parameters (i.e., all parameters except K_{OW}, K_M, chemical concentration in sediment, and chemical concentration in water) were entered into the model and tested using the other calibration chemicals. After confirming that these parameters performed well (i.e., had SPAFs less than 5) for other chemicals with a range of K_{OW}s (Section 5.3.3.1), these calibrated parameter values were applied to the models for all other modeled chemicals (Section 5.3.3.2). Probabilistic analysis was again used to select the values for chemical-specific parameters (K_{OW}, chemical concentration in water, and K_M~~metabolic rate constant~~s) associated with the best model performance (i.e., lowest SPAF) at the Study Area-wide average sediment concentration (see Section 5.3.5.2.2).

5.3.5.1 Comparison of Round 2 Model Predictions to Round 3 Data

Before recalibrating the model using all available data, the predicted tissue concentrations from the calibrated model developed as part of the Round 2 Report (Integral et al. 2007) were compared to the Round 3 tissue data per EPA comments (EPA 2008a). The majority

[12] Calibrated, non-chemical-specific parameters include general environmental parameters (OC content of sediment, concentration of suspended solids, water temperature, and dissolved organic carbon concentration in water) and species-specific parameters (weight, lipid fraction, water content, and dietary consumption fractions). See Appendix E for additional information.

of SPAFs calculated as part of this exercise were less than 5, with several exceptions where the Round 3 dataset was not representative of Study Area-wide conditions (e.g., crayfish and sculpin) or there were significant analytical differences between the two datasets. Appendix ~~F~~ D provides additional information regarding this comparison. The model development process is described in detail later in the section; however, it is noted that for all other applications of the model described here, data from all rounds of sampling were used together for model development and calibration.

5.3.5.2 Selection of Model Parameter Values and Distributions Used for Calibration

This section presents an overview of initial input values used in the probabilistic model (Appendix ~~D~~ B provides additional information on parameter distributions). The input parameters required by the adaptation of the Arnot and Gobas bioaccumulation model (Arnot and Gobas 2004) used in this report were derived from site-specific data whenever possible. The main sources of site-specific data were the Round 1 through 3 data collected for the Portland Harbor RI/FS. When an input parameter could not be defined using these data, literature values and best professional judgment were used.

For input into the model, parameter distributions were defined based on shape (i.e., normal, triangular, or uniform) and descriptive statistics (i.e., mean and standard deviation or nominal value, maximum, and minimum). The selected distributions were based on empirical data whenever possible and were intended to reflect the uncertainty surrounding estimates of central tendency. For example, in the central limit theorem, estimates of the mean (with sufficient sample size) approach a normal distribution. The standard deviation of the distribution of estimates of the mean is defined by the standard error of the original data. More information regarding all model parameter values and distributions is available in Appendix ~~D~~B. A summary of parameter values for chemical concentrations in sediment and water, K_{OW}, and K_M~~metabolic rate constant~~s are provided in this section.

Based on comments from EPA on the model developed as part of the Round 2 Report (Integral et al. 2007), 21 parameters calibrated as part of the Round 2 Report model were not calibrated for this version of the mechanistic model. These parameters include uptake constant A and B, the non-lipid organic matter (NLOM)-proportionality constant, and the species-specific dietary absorption efficiencies of lipid and NLOM, which are discussed further in Appendix ~~D~~B. Additionally, the sensitivity analysis performed as part of the Round 2 Report indicated that the model is generally not highly sensitive to these parameters,[13] and thus that the calibration of these parameters is not critical to refining model performance.

5.3.5.2.1 Chemical Concentrations in Water

Chemical concentrations in the water column for use in the mechanistic model were calculated using XAD water column samples collected during the seven sampling events at

[13] The one exception to this statement is the dietary absorption efficiency of lipids for epibenthic invertebrate consumers (EIC [crayfish]) had a large impact on the predicted EIC tissue concentration.

five transect locations. The averaging scheme used to develop mean and standard deviations used in the model (Table 5-2) is discussed in Appendix ~~D~~B.

Table 5-2. Chemical Concentrations in Surface Water

Analyte	Detection Frequency	Dissolved Water Concentration (ng/L)[a]	
		Mean	Standard Error
PCBs			
PCB 17	26/26	0.00434	0.000590
PCB 77	24/26	2.61×10^{-4}	3.90×10^{-5}
PCB 118	26/26	0.00282	0.000249
PCB 126	5/26	1.32×10^{-5}	1.04×10^{-6}
PCB 167	22/26	1.00×10^{-4}	8.22×10^{-6}
Total PCBs[b]	26/26	0.217	0.0244
~~**Dioxins and Furans**~~			
~~2,3,4,7,8-PeCDF~~	~~7/26~~	~~5.19×10^{-6}~~	~~5.97×10^{-7}~~
Pesticides			
4,4′-DDD	26/26	0.049	0.0090
4,4′-DDE	26/26	0.031	0.0028
4,4′-DDT	26/26	0.017	0.0021
Aldrin	23/26	0.0022	0.00022
alpha-HCH	26/26	0.027	0.0040
beta-HCH	20/26	0.0052	0.00042
Dieldrin	26/26	0.067	0.0092
gamma-HCH	26/26	0.025	0.0013
Heptachlor	3/26	0.00021	0.000016
Heptachlor epoxide	26/26	0.0071	0.00044
Sum DDD	26/26	0.070	0.013
Sum DDE	26/26	0.032	0.0029
Sum DDT	26/26	0.022	0.0024
Total chlordane	26/26	0.029	0.0019
Total DDx	26/26	0.13	0.017

[a] The standard error of the data were used to describe the standard deviation of estimates of the mean.
[b] Sum of PCB congeners.
DDD – dichlorodiphenyldichloroethane
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane

HCH – hexachlorocyclohexane
PCB – polychlorinated biphenyl
~~PeCDF – pentachlorodibenzofuran~~
total DDx – sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE and 4,4′-DDT)

5.3.5.2.2 Chemical Concentrations in Sediment

Sediment chemistry data were available from LWG and non-LWG sources for locations throughout the Study Area (RM 2 to RM 11). In order to minimize any spatial bias that may be present in the data, a SWAC was calculated for the modeled chemicals using the natural neighbors approach for Study Area-wide exposure estimates (Table 5-3).

Table 5-3. Spatially Weighted Average Concentrations for Chemicals in Sediment

Chemical	Detection Frequency	Natural Neighbors SWAC (µg/kg dw)
PCBs		
PCB 17	246/253	1.07
PCB 77	254/266	0.185
PCB 118	40/96	3.28
PCB 126	251/266	0.0175
PCB 167	264/266	0.230
Total PCBs[a]	872/1,103	92.6
~~**Dioxins and Furans**~~		
~~2,3,4,7,8-PeCDF~~	~~173/219~~	~~0.0115~~
Pesticides		
4,4´-DDD	951/1,128	6.26
4,4´-DDE	928/1,125	3.43
4,4´-DDT	769/1,113	14.8
Aldrin	252/1,034	0.466
alpha-HCH	206/1,072	0.267
beta-HCH	443/1,083	1.28
Dieldrin	246/1,078	0.536
gamma-HCH	182/1,083	0.706
Heptachlor	72/1,083	0.216
Heptachlor epoxide	87/1,082	0.290
Sum DDD	969/1,128	8.89
Sum DDE	933/1,125	4.22
Sum DDT	856/1,127	17.3
Total chlordane	734/1,083	2.40
Total DDx	1,021/1,128	30.3

[a] Total PCBs were calculated as the sum of congeners, when available. When congener data were not available, the sum of Aroclors data was used.

COC – chemical of concern
DDD – dichlorodiphenyldichloroethane
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
dw – dry weight
HCH – hexachlorocyclohexane
PCB – polychlorinated biphenyl
~~PeCDF – pentachlorodibenzofuran~~
SWAC – spatially weighted average concentration
total DDx – sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE and 4,4′-DDT)

Sediment chemistry data were available from LWG and non-LWG sources for locations throughout the Study Area (RM 2 to RM 11). In order to minimize any spatial bias that may be present in the data, a SWAC was calculated for the modeled chemicals using the natural neighbors approach for Study Area-wide exposure estimates (Table 5-3).

The process for developing natural neighbors SWACs is described in Appendix ~~D~~B.

The mechanistic model was applied on a Study Area-wide basis for calibration, using the Study Area-wide SWAC value to represent the sediment exposure concentration for all modeled organisms and the Study Area-wide average tissue concentrations (by species) to represent the tissue concentrations associated with the Study Area-wide SWAC. The Study Area-wide SWAC was assumed to represent the average sediment exposure condition for the sampled organisms. This could be a source of error for small-home-range species collected from areas of known or suspected sediment contamination (e.g., crayfish) because the Study Area-wide SWAC might underestimate the average sediment exposure condition for the sampled organisms (which would result in an overestimation of bioaccumulation and conservatively biased PRGs for that species). For developing PRGs using the model, sediment chemical concentration was defined as a decision variable, consistent with Morgan and Henrion (1990). According to Morgan and Henrion (1990), sediment chemical concentrations should be treated parametrically because they are decision variables. “Treated parametrically” means that the SWAC should not be used as a calibration parameter.

In order to calibrate the model, it was necessary to define current conditions (Table 5-3). Uncertainties surrounding estimates of the baseline (current conditions) SWAC would also apply to alternative conditions (such as PRGs or estimates of post-remediation SWACs) provided they all are calculated consistently (i.e., based on the same natural neighbors interpolation method). This does not mean that sediment concentration uncertainty can be ignored, but it reduces the importance of this uncertainty in the model. Uncertainty associated with this assumption was explored through the model sensitivity and uncertainty analysis but was not included in the model calibration (unlike water chemical concentrations, whose distributions were used for model calibration).

5.3.5.2.3 Octanol-Water Partition Coefficient

For each chemical that was modeled, the literature was searched to compile possible K_{OW} values, as discussed in Appendix ~~D~~B. Uniform distributions were used when calibrating the model, defined by a nominal value and a minimum and maximum from the literature sources. For those chemicals that were modeled individually (e.g., PCB 126 and 4,4′-DDT), these values were selected directly from the literature sources. For the chemical mixtures that were modeled (e.g., total PCBs and total DDx), K_{OW} values were weighted based on the percent contribution of the individual components before selecting distribution values (see Appendix ~~D~~ B for more information). Table 5-4 shows the nominal value and uniform distribution values that were used to calibrate the model.

Table 5-4. K_{OW} Values for Use in the Model

	log K_{OW} Values	
Analyte	**Nominal Value**	**Distribution Range**
PCBs		
PCB 17	5.70	4.60 – 5.76
PCB 77	6.22	5.62 – 7.87
PCB 118	6.85	6.24 – 7.42
PCB 126	6.83	6.38 – 7.00
PCB 167	7.48	6.82 – 7.62
Total PCBs[a]	7.40	6.09 – 7.84
~~**Dioxins and Furans**~~		
~~2,3,4,7,8-PeCDF~~	~~6.95~~	~~6.56 – 7.82~~
Pesticides		
4,4′-DDD	6.05	4.82 – 6.33
4,4′-DDE	6.90	4.28 – 6.97
4,4′-DDT	6.72	3.98 – 8.31
Aldrin	6.39	3.01 – 7.50
alpha-HCH	3.78	3.19 – 4.57
beta-HCH	3.78	3.19 – 4.26
Dieldrin	5.37	2.60 – 6.20
gamma-HCH	3.73	3.19 – 4.26
Heptachlor	6.03	3.87 – 6.10
Heptachlor epoxide	5.29	3.65 – 5.42
Sum DDD	6.00	4.80 – 6.31
Sum DDE	6.80	4.22 – 6.87
Sum DDT	6.58	3.98 – 8.19
Total DDx	6.65	4.34 – 7.08
Total chlordane	6.42	2.78 – 6.42

[a] The total PCB K_{OW} values are based only on data for total PCBs as congeners (not Aroclors). K_{OW} weighting was done based on all available field-collected tissue data (invertebrates and fish). See Appendix ~~D~~ B for additional information.

DDD – dichlorodiphenyldichloroethane

K_{OW} – octanol-water partition coefficient

DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
HCH – hexachlorocyclohexane
PCB – polychlorinated biphenyl
~~PeCDF – pentachlorodibenzofuran~~
total DDx – sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE and 4,4′-DDT)

5.3.5.2.4 Metabolic Rate Constant

Chemical-specific metabolism is one of the four chemical elimination routes in the Arnot and Gobas food web model (Arnot and Gobas 2004).[14] The metabolism, or biotransformation, of some chemicals explains why they are not bioaccumulated in the tissues of higher trophic level organisms to the extent that would be predicted. A review of literature regarding ~~metabolic rate constants (~~K_Ms~~)~~ indicates that some members of the chemical classes being modeled for Portland Harbor are likely metabolized (e.g., Niimi 1996; Sijm et al. 1993; Opperhuizen and Sijm 1990; Konwick et al. 2006).

Table 5-5 presents the K_M~~metabolic rate constant~~s for chemicals identified in Appendix ~~D~~ B as being metabolized to a significant extent (i.e., metabolism occurs at a rate such that acceptable model performance cannot be achieved without the inclusion of metabolism). As discussed in Appendix ~~D~~B, a uniform distribution was used for model calibration, with values based on Arnot et al. (2008). For chemicals not listed in this table, no metabolism was assumed in the mechanistic model.

Table 5-5. Metabolic Rate Constants (1/day) for Metabolized Chemicals

Chemical	Selected K_M Values: Nominal Value	Selected K_M Values: Distribution Range
PCBs		
PCB 77	0.03	0 – 0.3
PCB 126	0.003	0 – 0.03
~~**Dioxins and Furans**~~		
~~2,3,4,7,8-PeCDF~~	~~0.03~~	~~0 – 0.3~~
DDTs		
4,4′-DDT	0.01	0 – 0.1
Sum DDT[b]	0.005[b]	0 – 0.05[b]

Source: Arnot et al. (2008)

[a] As a conservative estimate, the metabolic rate for sum DDT was estimated as equal to one-half of the metabolic rate selected for 4,4′-DDT, although 4,4′-DDT made up more than 50% of sum DDT. Sum DDT is the sum of 2,2′-DDT and 4,4′-DDT. The former is not expected to metabolize significantly.

DDT – dichlorodiphenyltrichloroethane
K_M – metabolic rate constant
PCB – polychlorinated biphenyl
~~PeCDF – pentachlorodibenzofuran~~

[14] The other three routes by which chemical concentrations in tissue may decrease are through respiratory (gill) elimination, fecal egestion, and growth dilution (Arnot and Gobas 2004).

5.3.5.3 Probabilistic Approach to Model Calibration

In order to calculate PRGs, it was necessary to develop a calibrated model. Calibration was performed by selecting the input parameter values from initial parameter distributions that produced the best estimate of the smallmouth bass empirical tissue concentration while also closely predicting the empirical tissue concentrations of the other modeled species. Empirical tissue concentrations for modeled chemicals that were used to calculate SPAFs are presented in Appendix ~~G~~E.

The calibration process is shown in Figure 5-1 and described in detail in the subsections that follow. This process was performed in two steps. First, the model was calibrated for the parameters applicable to all chemicals (i.e., non-chemical-specific parameters), and then for each chemical, the model was further calibrated for those parameters that were chemical-specific (i.e., K_{OW}, chemical concentration in water, and K_M~~metabolic rate constant~~). The SWAC was used as a point estimate for the sediment chemical concentration. Because the uncertainty surrounding current sediment chemical concentrations would also apply to alternative conditions (PRGs), a distribution describing many of the uncertainties surrounding the SWAC was not included in the model calibration. The SWAC is not used as a calibration parameter though because that would make using PRGs (and RGs) much more complicated. For example, assume that a SWAC had an estimated value of 15, with an uncertainty range of 10 to 20. Assume that the calibrated SWAC value was 12, which represented the 20th percentile of the SWAC uncertainty distribution. The PRG would then be based on the 20th percentile of the uncertainty distribution on the SWAC, rather than on the straight spatially weighted average sediment concentration. This would make hilltopping exercises and post-remediation monitoring unnecessarily complicated because instead of just determining whether the SWAC had been achieved, one would have to determine that the 20th percentile of the SWAC uncertainty distribution had been achieved.

In addition, uncertainty related to the relationship between sediment chemical concentrations and other parameters, such as water chemical concentration, were not evaluated through the inclusion of distributions. The uncertainties related to sediment chemical concentrations and the contribution of sediment and water to model-predicted tissue concentrations are evaluated in the uncertainty analysis. However, the bioaccumulation model treats water and sediment concentrations as inputs. It does not model abiotic fate and transport processes that govern the contribution of sediment and water to model-predicted tissue concentrations. That analysis also is important for understanding the relative contribution of sediment versus other sources to tissue concentrations and is a topic for the hybrid model that is being developed for the FS.

Non-Chemical-Specific Calibration

1. Model was first run probabilistically 50,000 times with total PCBs (K_{ow} = 7.40)
2. All parameters were allowed to vary with the exception of the sediment concentration, which was held constant.[1]
3. Model output was sorted based on the SPAF for smallmouth bass, and the top 25 model runs were selected while also optimizing the SPAFs for other species.
4. The model was then run deterministically with these 25 parameter sets to evaluate the model's ability to predict on a smaller spatial scale for individual smallmouth bass composite samples. The top 4 parameter sets were selected.
5. The model was then run deterministically for these four parameter sets for the five additional calibration chemicals (PCB 17, PCB 118, PCB 167, 4,4′-DDE, and total DDTs)[2], both on a site-wide basis and for smallmouth bass on a smaller spatial scale.
6. The best parameter set was selected. As with total PCBs, the model performance improved with the use of the calibrated parameter values.

Chemical-Specific Calibration

1. The model was parameterized with all of the non-chemical-specific calibrated values.
2. Chemical-specific parameter values for chemical concentration in sediment, chemical concentration in water, K_{ow}, and metabolic rate constant were entered into the model.
3. Distributions were defined for the chemical-specific K_{ow} and water concentration and the model was run probabilistically 1,000 times.
4. The model output was sorted based on the SPAF for smallmouth bass, while also optimizing the SPAFs for other species. The best model run was used to select the calibrated K_{ow} and water concentration.
5. For chemicals known to be metabolized, the calibrated K_{ow} and water concentration were entered into the model, and distributions were defined for the metabolic rate constants before again probabilistically running the model 1,000 times.
6. Again, the model output was sorted based on the SPAF for smallmouth bass, while also optimizing the SPAFs for other species. The best model run was used to select the calibrated metabolic rate constants.

[1] When PRGs were calculated, the actual sediment concentration was not used, and thus the calibration of this parameter was not necessary.
[2] Uncalibrated chemical-specific parameters (chemical concentration in water, chemical concentration in sediment, and K_{ow}) were used for this assessment.

Figure 5-1. Mechanistic Model Calibration Process

5.3.5.3.1 Calibration of Non-Chemical-Specific Parameters

The calibration of the model for non-chemical-specific parameters was performed first, using all available data, this includes data collected as part of Rounds 1, 2, and 3 (as discussed in Section 3.1).

Step 1. Initial Calibration Model Run for Total PCBs

For the initial calibration of non-chemical-specific parameters~~In this case~~, total PCBs was selected ~~for~~ as the primary chemical ~~the initial calibration~~ (see Section 5.3.3.1). The model was run probabilistically 50,000 times using the parameter distributions derived from site-specific data and literature values (performed using Crystal Ball-® software) (see Appendix ~~D~~B). Both chemical-specific and non-chemical-specific parameters were allowed to vary to ensure that the calibrated parameters were not overly constrained. The only exception was that sediment concentration was held as a point estimate, as explained previously.

Step 2. Elimination of Runs with Parameter Values Outside of Specified Ranges

A screening step was performed on the 50,000 iterations to eliminate runs for which the invertebrate and fish dietary percentages fell outside of the acceptable ranges~~After the model had been run 50,000 times, a screening step was performed to confirm that no parameters fell outside of the acceptable range~~ (species-specific dietary ranges and rationale are further discussed in ~~i.e., the ranges defined as distributions of mean estimates for parameters in~~ Appendix ~~D~~B). This step was necessary because for each model run, the sum~~total~~ of the randomly selected dietary fractions was normalized to equal 1 (i.e., 100%), meaning that it was possible to generate dietary fractions outside of the initial specified ranges. Eliminating runs for which ~~whose~~ parameters fell outside of the acceptable ranges was done to ensures~~This was important for the dietary parameters because it was necessary to normalize these values to ensure~~ that the calibrated model includes realistic dietary assumptions for each modeled trophic group~~ was achieving the correct total food intake~~. ~~Dietary intake for each trophic group was defined by ranges of fractional consumption of sediment and other organisms. For each model iteration, the total of the randomly selected dietary fractions was normalized to equal 1. During the normalization process, it is possible to generate dietary fractions outside the initial specified ranges (see Appendices D and E for details on diet).~~

Step 3. Elimination of Runs Based on SPAFs for Modeled Species

The remaining acceptable model runs (n = 9,982) were ~~sorted~~ filtered based on the SPAF for modeled fish and invertebrate species: ~~smallmouth bass.~~

- ~~Model runs with~~ Model runs with SPAFs greater than 1.5 for smallmouth bass were discarded (842 model runs remained).

- ~~The remaining model runs (n = 842) were further limited by discarding any model runs with~~ Model runs with SPAFs greater than 5 for carp were discarded (168 model runs remained).[15]

- Model runs with SPAFs greater than 2~~3~~ for other fish species (i.e., sculpin, largescale sucker, and northern pikeminnow) were discarded (61 model runs remained).

- ~~and/or~~ Model runs with SPAFs greater than 5 for invertebrates (i.e., BIF and EIC) were discarded (25 model runs remained).

The remaining~~se~~ 25 qualifying model runs were selected for additional analysis. The result of this calibration process was a model that is highly accurate for smallmouth bass while still predicting well for other modeled species.

Step 4. Evaluation of Model at Smaller Spatial Scales

The non-chemical-specific parameter values from these top 25 model runs (i.e., parameter sets) were then used to evaluate the model's ability to predict smallmouth bass tissue concentrations on a smaller spatial scale (using 1-RM SWACs) for total PCBs. This evaluation was done using ~~T~~the non-chemical-specific parameters from the top 25 model runs and nominal values for chemical-specific parameters (i.e., K_{OW} and chemical concentration in water) were used along with estimates of sediment concentrations for each bass composite sample (see Section 3.3.3) to estimate smallmouth bass tissue concentrations for individual composites. SPAFs were then calculated for each composite sample, and an average SPAF across the individual composite samples was calculated for each of the 25 parameter sets. Before selecting the top model runs, consideration was also given to key parameter values. The range of mean surface water temperature values based on the available empirical data was determined to likely be outside of the range of reasonable values. Thus, parameter sets with water temperatures more than 1 ºC off of the average empirical value of 13.9 ºC (i.e., < 12.9 or > 14.9 ºC) were excluded from consideration. Of the remaining 10 parameter sets, ~~and~~ the best four model runs (sorted based on the SPAF for smallmouth bass) were carried forward to the next step.

Step 5. Evaluation of Model for Other Calibration Chemicals

To further evaluate ~~T~~the four selected model runs, these parameter sets were ~~then~~ evaluated for the other five calibration chemicals (PCB 17, PCB 118, PCB 167, 4,4′-DDE, and total DDx). As with total PCBs, these model runs were evaluated both on a Study-Area-wide basis and on a smaller spatial scale for smallmouth bass.~~, again using~~ For this evaluation,

[15] The SPAF for carp was higher than that for other fish species for total PCBs because of the presence of two high values in the dataset. When these values were excluded, the carp SPAFs for the selected 25 model runs were all less than 2.

nominal values were used for chemical-specific parameters (i.e., K_{OW}, chemical concentration in sediment, and chemical concentration in water).[16] ~~From the results of this exercise, the best model run was selected.~~

Empirical invertebrate and fish tissue data for each calibration chemical were compared ~~to~~ with the model-predicted tissue concentrations, using both the uncalibrated and calibrated non-chemical-specific parameters to ensure that calibration had improved model performance (i.e., generally reduced the SPAF). The final calibrated parameter set was identified based on the following:

- **Site-wide model performance** – Model runs were sorted based on the average SPAF for the seven species (i.e., the five fish species and two invertebrate species) across the five calibration chemicals on a site-wide basis.
- **Smallmouth bass smaller-spatial-scale model performance** – Model runs were sorted based on the average SPAF across smallmouth bass composite samples and across the five calibration chemicals.

The same model run was identified using both of the above metrics (i.e., site-wide and smaller-spatial-scale performance), and thus the parameter set associated with this model run was selected. These parameter values ~~in the selected model run~~ were then accepted as final calibrated values for the non-chemical-specific parameters.

5.3.5.3.2 Calibration of Chemical-Specific Parameters

Once the non-chemical-specific parameters had been calibrated, the next step was to calibrate the model for each chemical needed for PRG calculations. Chemical-specific parameters include the K_{OW}, the chemical concentration in water, the chemical concentration in sediment, and the K_M~~metabolic rate constant~~. As with the non-chemical-specific parameter calibration, the sediment concentration (Study Area-wide SWAC) was held as a constant.

The chemical-specific calibration was done in two steps. The first step was to determine a calibrated value for t~~T~~he K_{OW} and chemical concentration in water. ~~were defined in the first step, and then,~~ The second step was to determine a calibrated value for ~~those chemicals known to be metabolized,~~ the K_M~~metabolic rate constant~~ for chemicals known to be metabolized~~. was calibrated in the second step~~. This two-step calibration process was done to ensure that the K_M~~metabolic rate constant~~ calibration did not influence the calibration of K_{OW} or water concentration. For each chemical, the ~~non-chemical-specific~~ calibrated values for all non-chemical-specific parameters were entered into the model, and distributions were defined for the chemical's K_{OW} and concentration in water (see Section 5.3.5.2 and Appendix ~~D~~ B for details on distribution selection).

[16] The selected calibration chemicals are not thought to be metabolized to a significant extent. The selection of non-metabolized chemicals was intentional to ensure that model calibration was not impacted by metabolism.

Step 1. Calibration of Chemical-Specific K_{OW} and Concentration in Water

In this first step, ~~For those chemicals known to be metabolized, the~~a nominal value for the K_M~~metabolic rate constant~~ ~~was entered~~ was entered into the model. ~~, but n~~No distribution was defined for the K_M in this first step to ensure that the metabolic rate calibration did not influence the calibration of K_{OW} and water concentration. The model was then run 1,000 times for each chemical, and the ~~model~~ output was sorted based on the SPAFs for smallmouth bass. Other considerations for selecting a calibrated value for ~~T~~the K_{OW} and chemical concentration included the following:

- SPAFs for smallmouth bass were < 2, and the percent difference for smallmouth bass was considered to ensure that the model was not under-predicting concentrations for this important species.
- SPAFs for other fish species were considered, and model runs were also sorted to optimize model performance for these species (SPAFs generally < 3).
- Consistency with the K_{OW} values used in the contaminant fate and transport model and with values expected based on the component chemicals were also considered when applicable (i.e., when chemicals were modeled both in the fate and transport model and in the bioaccumulation model).

~~in water were selected based on improving the SPAF for smallmouth bass (SPAFs < 2) while also optimizing the SPAFs for the other species (SPAFs generally < 3).~~The result of this calibration process was the selection of realistic ~~a~~ calibrated K_{OW} values and chemical concentrations in water that improved the model performance for smallmouth bass and other species.

Step 2. Calibration of Chemical-Specific Metabolic Rates

The second step, which was conducted only for chemicals known to be metabolized, included using ~~For chemicals known to be metabolized,~~ the calibrated K_{OW} and chemical concentration in water ~~were entered~~ in~~to~~ the model. ~~and~~ Next, uniform distributions (representing uncertainty ranges) were ~~then~~ defined for the K_M~~metabolic rate constant~~s (see Section 5.3.5.2 and Appendix ~~D~~ B for details on distribution selection). The model was again run 1,000 times for each chemical, and the output was evaluated using the same criteria described in Step 1. ~~and the~~ The calibrated K_M~~metabolic rate constant~~s were selected to ~~based on optimizing~~ improve~~ing~~ model performance for smallmouth bass (SPAFs < 1.5) while also improving model performance for the other species (SPAFs generally < 3).

Inherent in this calibration process is the assumption that the basic model structure is correct (i.e., the biological processes included in the model, the trophic groups included, and the relative relationships of the trophic groups are defined appropriately). With all parameters calibrated, the minimum acceptable model performance was a SPAF of ≤ 3 for smallmouth bass, and a SPAF of ≤ 10 for all other species-chemical combinations.

5.4 PREDICTIVE MODEL RESULTS

This section presents the model calibration results for non-chemical-specific and chemical-specific parameters, calibrated model performance, and a brief discussion of the human health and ecological PRG development. PRGs were presented in the Early PRG Report (Windward et al. 2009).

5.4.1 Calibration for Non-Chemical-Specific Parameters

As discussed in Section 5.3.5, the model was first calibrated for non-chemical-specific parameters using calibration chemicals with a range of K_{OW}s (5.70 to 7.48 for the selected calibration chemicals). The non-chemical-specific calibrated parameter values were selected from the best-performing model run across all of the calibration chemicals (total PCBs, PCB 17, PCB 118, PCB 167, 4,4′-DDE, and total DDx) and both on a Study Area-wide basis and for individual smallmouth bass composite samples on a smaller spatial scale. Table 5-6 presents the SPAF for each of the calibration chemicals using the initial uncalibrated parameter values (i.e., the nominal value of the distributions) and the calibrated parameter values. Note that at this point, the model used uncalibrated ~~(i.e., nominal)~~ values for ~~chemical-specific parameters (i.e.,~~ chemical concentration in water and K_{OW}~~)~~. For all calibration chemicals, the SWAC was used for the sediment chemical concentration. The SPAFs for all species with available empirical data are presented in Table 5-6.

Table 5-6. SPAFs for Calibration Chemicals Based on Calibrated Non-Chemical-Specific Parameters and Uncalibrated Chemical-Specific Parameters

Parameter Set	SPAFs[a]							Average SPAF
	BIF	EIC	SCL	LSS	CAR	SMB	NPM	
Total PCBs								
Uncalibrated	3.9	**(4.4)**	**(1.3)**	**(1.1)**	3.3	**(3.8)**	**(2.6)**	2.9
Post-calibration[b]	3.1	**(3.7)**	**(1.1)**	1.0	3.0	**(2.5)**	**(2.1)**	2.4
PCB 17								
Uncalibrated	4.9	**(10.0)**	**(1.1)**	NA	**(1.6)**	**(5.1)**	NA	4.5
Post-calibration[b]	4.3	**(8.7)**	**(1.1)**	NA	1.4	**(3.9)**	NA	3.9
PCB 118								
Uncalibrated	3.2	**(2.3)**	**(1.4)**	NA	**(1.6)**	**(6.9)**	NA	3.1
Post-calibration[b]	2.5	**(1.9)**	**(1.2)**	NA	**(1.8)**	**(4.5)**	NA	2.4
PCB 167								
Uncalibrated	8.0	1.2	1.1	NA	4.0	**(2.4)**	NA	3.3
Post-calibration[b]	6.1	1.4	1.4	NA	3.6	**(1.5)**	NA	2.8
4,4′-DDE								
Uncalibrated	3.8	**(2.8)**	**(1.2)**	1.5	1.9	**(2.8)**	1.5	2.2
Post-calibration[b]	3.3	**(2.6)**	**(1.1)**	1.6	1.7	**(2.0)**	1.6	2.0
Total DDx								

Table 5-6. SPAFs for Calibration Chemicals Based on Calibrated Non-Chemical-Specific Parameters and Uncalibrated Chemical-Specific Parameters

Parameter Set	SPAFs[a]							Average SPAF
	BIF	EIC	SCL	LSS	CAR	SMB	NPM	
Uncalibrated	2.0	**(7.5)**	**(2.0)**	**(1.8)**	**(2.1)**	**(9.2)**	**(3.2)**	4.0
Post-calibration[b]	1.7	**(6.5)**	**(1.8)**	**(1.7)**	**(2.4)**	**(6.3)**	**(2.9)**	3.3

[a] (**SPAFs)** shown in **bold** and in parentheses indicate that the model was over-predicting for this species-chemical combination.

[b] Calibrated values were used for non-chemical specific parameters. Nominal values were used for the chemical-specific parameters.

BIF – benthic invertebrate filter feeder (clams)
CAR – carp
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
EIC – epibenthic invertebrate consumer (crayfish)
LSS – largescale sucker
NA – not available
NPM – northern pikeminnow
PCB – polychlorinated biphenyl
SCL – sculpin
SMB – smallmouth bass
SPAF – species predictive accuracy factor
total DDx – sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE and 4,4′-DDT)

In most cases, the use of the calibrated non-chemical-specific parameters reduced the SPAFs (i.e., improved model performance) for the modeled species. For the six chemical-species combinations where the SPAF increased, the increases were no greater than 0.3, and the post-calibration SPAFs were still < 2.5. Even without the calibration of the chemical-specific parameters, most chemical-species combinations had SPAFs < 5, and all had SPAFs < 10. Overall, the calibration reduced both over- and under-prediction for most chemical-trophic group combinations, and the average SPAF for each chemical was decreased when the calibrated non-chemical-specific parameters were used.

Additionally, to evaluate the model on a smaller spatial scale, the model performance for individual smallmouth bass samples was examined, and is shown in Table 5-7.

Table 5-7. SPAFs for Calibration Chemicals for Smallmouth Bass

	Using Mean 1-RM SWAC			Using Minimum 1-RM SWAC			Using Maximum 1-RM SWAC		
Parameter Set	Average SPAF	Count SPAF<5	Count SPAF<10	Average SPAF	Count SPAF<5	Count SPAF<10	Average SPAF	Count SPAF<5	Count SPAF<10
Total PCBs									
Uncalibrated	6.1	16 of 32	28 of 32	3.8	27 of 32	31 of 32	10.5	9 of 32	22 of 32
Post-calibration[a]	3.9	24 of 32	30 of 32	2.6	31 of 32	31 of 32	6.7	20 of 32	26 of 32
PCB 17									
Uncalibrated	7.7	18 of 32	27 of 32	3.1	28 of 32	30 of 32	16.1	14 of 32	20 of 32
Post-calibration[a]	5.9	23 of 32	28 of 32	2.6	29 of 32	32 of 32	12.2	18 of 32	22 of 32
PCB 118									
Uncalibrated	18.0	8 of 32	19 of 32	5.1	21 of 32	27 of 32	40.2	6 of 32	11 of 32
Post-calibration[a]	11.6	14 of 32	22 of 32	3.4	26 of 32	28 of 32	25.9	8 of 32	20 of 32
PCB 167									
Uncalibrated	3.6	26 of 32	31 of 32	2.5	30 of 32	31 of 32	6.5	19 of 32	30 of 32
Post-calibration[a]	2.4	31 of 32	31 of 32	2.4	28 of 32	30 of 32	4.1	25 of 32	30 of 32
4,4′-DDE									
Uncalibrated	3.6	27 of 32	31 of 32	2.6	30 of 32	32 of 32	5.0	22 of 32	29 of 32
Post-calibration[a]	2.6	30 of 32	32 of 32	2.0	32 of 32	32 of 32	3.4	25 of 32	31 of 32
Total DDx									
Uncalibrated	15.2	3 of 32	17 of 32	7.4	12 of 32	26 of 32	25.8	2 of 32	14 of 32
Post-calibration[a]	10.4	10 of 32	22 of 32	5.3	19 of 32	29 of 32	17.3	8 of 32	17 of 32

[a] Calibrated values were used for non-chemical-specific parameters. Nominal values were used for the chemical-specific parameters except for the chemical concentration in sediment. As described in Section 3.3.3, 1-RM SWACs were calculated for each fish in the bass composite and were used to estimate the sediment concentration to which the fish were exposed.

DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
PCB – polychlorinated biphenyl
RM – river mile
SPAF – species predictive accuracy factor
SWAC – spatially weighted average concentration
total DDx – sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE and 4,4′-DDT)

As shown in Table 5-7, the use of the calibrated parameter set for the non-chemical-specific parameters in the model improved the average SPAF across smallmouth bass composites using the mean, minimum, or maximum SWAC. Additionally, in all cases the number of samples with SPAFs < 5 and those < 10 increased when the calibrated parameter set was used. Based on this analysis, the model was determined to be fully calibrated for non-chemical-specific parameters.

Tables 5-8 through 5-11 provide the original distributions as well as the selected calibrated values for non-chemical-specific parameters. Table 5-8 shows the environmental parameters, Table 5-9 shows the general biological parameters, Table 5-10 shows the species-specific biological parameters, and Table 5-11 shows the dietary parameters that were used in the model. Information concerning the selection of the initial distributions can be found in Appendix ~~D~~B.

Table 5-8. Calibrated Values for Environmental Parameters

Model Component	Unit	Initial Distribution[a]	Calibrated Value
Water temperature	°C	13.9 (SD = 1.7)	13.7
Concentration of TSS	kg/L	1.13×10^{-5} (SD = 4.5×10^{-6})	1.4×10^{-5}
DOC concentration in water	kg/L	1.38×10^{-6} (SD = 5.9×10^{-8})	1.31×10^{-6}
Organic carbon content of sediment	Fraction	0.0171 (SD = 0.00028)	0.0171

[a] A normal distribution was assigned with the first value as the mean and the indicated standard deviation.
DOC – dissolved organic carbon
SD – standard deviation
TSS – total suspended solids

Table 5-9. Calibrated Values for General Biological Parameters

Model Component	Model Symbol	Nominal Value (unitless)[a]
Resistance to chemical uptake through aqueous phase for phytoplankton/algae	UA	6.0×10^{-5}
Resistance to chemical uptake through organic phase for phytoplankton/algae	UB	5.5
Dietary transfer efficiency constant A	EDA	3.0×10^{-7}
Dietary transfer efficiency constant B	EDB	2.0
NLOM-octanol proportionality constant	BETA	0.035
NLOC-octanol proportionality constant	GAMMA	0.35

[a] No distributions were defined for these parameters, as discussed in Appendix ~~D~~B.
NLOC – non-lipid organic carbon
NLOM – non-lipid organic matter

Table 5-10. Calibrated Values for Species-Specific Biological Parameters

Model Component	Unit	Distribution Type	Initial Distribution[a]	Calibrated Value
Phytoplankton/algae				
Lipid content	Fraction	Triangle	0.00123 (0.0008 – 0.002)	0.00123
Moisture content	Fraction	Triangle	0.955 (0.935 – 0.993)	0.947
Fraction of porewater ventilated	Fraction	Point estimate	0	0
Growth rate constant	1/day	Triangle	0.08 (0.03 – 0.13)	0.09
Zooplankton				
Weight	kg	Triangle	1.4×10^{-7} ($3.3 \times 10^{-8} – 2.3 \times 10^{-7}$)	1.7×10^{-7}
Lipid content	Fraction	Triangle	0.01 (0.009 – 0.011)	0.011
Moisture content	Fraction	Triangle	0.90 (0.80 – 0.98)	0.82
Dietary absorption efficiency of lipid	Fraction	Point estimate	0.72	0.72
Dietary absorption efficiency of NLOM	Fraction	Point estimate	0.72	0.72
Dietary absorption efficiency of water	Fraction	Point estimate	0.25	0.25
Fraction of porewater ventilated	Unitless	Point estimate	0	0
Benthic Invertebrate Filter Feeders (clams)				
Weight	kg	Normal	0.00125 (SD = 1.3×10^{-5})	0.00126
Lipid content	Fraction	Normal	0.022 (SD = 0.0011)	0.02225
Moisture content	Fraction	Normal	0.86 (SD = 0.0029)	0.863
Dietary absorption efficiency of lipid	Fraction	Point estimate	0.75	0.75
Dietary absorption efficiency of NLOM	Fraction	Point estimate	0.75	0.75
Dietary absorption efficiency of water	Fraction	Point estimate	0.25	0.25
Fraction of porewater ventilated	Unitless	Uniform	0.05 (0.01 – 0.10)	0.05
Filter feeder scavenging efficiency	Unitless	Point estimate	1.0	1.0
Benthic Invertebrate Consumers				
Weight	kg	Triangle	5.33×10^{-6} ($1.4 \times 10^{-6} – 6.0 \times 10^{-6}$)	4.80×10^{-6}
Lipid content	Fraction	Triangle	0.015 (0.008 – 0.042)	0.014
Moisture content	Fraction	Triangle	0.80 (0.72 – 0.88)	0.80
Dietary absorption efficiency of lipid	Fraction	Point estimate	0.75	0.75
Dietary absorption efficiency of NLOM	Fraction	Point estimate	0.75	0.75
Dietary absorption efficiency of water	Fraction	Point estimate	0.25	0.25
Fraction of porewater ventilated	Unitless	Uniform	0.01 – 0.10	0.07

Table 5-10. Calibrated Values for Species-Specific Biological Parameters

Model Component	Unit	Distribution Type	Initial Distribution[a]	Calibrated Value
Epibenthic Invertebrate Consumers (crayfish)				
Weight	kg	Normal	0.0435 (SD = 0.00071)	0.0438
Lipid content	Fraction	Normal	0.0078 (SD = 0.00045)	0.00762
Moisture content	Fraction	Normal	0.74 (SD = 0.0031)	0.738
Dietary absorption efficiency of lipid	Fraction	Point estimate	0.75	0.75
Dietary absorption efficiency of NLOM	Fraction	Point estimate	0.75	0.75
Dietary absorption efficiency of water	Fraction	Point estimate	0.25	0.25
Fraction of porewater ventilated	Unitless	Uniform	0.01 – 0.10	0.03
Sculpin				
Weight	kg	Normal	0.0196 (SD = 0.00039)	0.01997
Lipid content	Fraction	Normal	0.041 (SD = 0.0016)	0.0416
Moisture content	Fraction	Normal	0.75 (SD = 0.0023)	0.751
Dietary absorption efficiency of lipid	Fraction	Point estimate	0.92	0.92
Dietary absorption efficiency of NLOM	Fraction	Point estimate	0.60	0.60
Dietary absorption efficiency of water	Fraction	Point estimate	0.25	0.25
Fraction of porewater ventilated	Fraction	Uniform	0.01 – 0.10	0.04
Largescale Sucker				
Weight	kg	Normal	0.794 (SD = 0.012)	0.8039
Lipid content	Fraction	Normal	0.076 (SD = 0.0052)	0.0733
Moisture content	Fraction	Normal	0.71 (SD = 0.0054)	0.714
Dietary absorption efficiency of lipid	Fraction	Point estimate	0.92	0.92
Dietary absorption efficiency of NLOM	Fraction	Point estimate	0.60	0.60
Dietary absorption efficiency of water	Fraction	Point estimate	0.25	0.25
Fraction of porewater ventilated	Unitless	Point estimate	0	0
Common Carp				
Weight	kg	Normal	2.48 (SD = 0.066)	2.50
Lipid content	Fraction	Normal	0.088 (SD = 0.0053)	0.0935
Moisture content	Fraction	Normal	0.69 (SD = 0.0047)	0.684
Dietary absorption efficiency of lipid	Fraction	Point estimate	0.92	0.92
Dietary absorption efficiency of NLOM	Fraction	Point estimate	0.60	0.60
Dietary absorption efficiency of water	Fraction	Point estimate	0.25	0.25
Fraction of porewater ventilated	Unitless	Point estimate	0	0

Table 5-10. Calibrated Values for Species-Specific Biological Parameters

Model Component	Unit	Distribution Type	Initial Distribution[a]	Calibrated Value
Smallmouth Bass				
Weight	kg	Normal	0.395 (SD = 0.18)	0.3524
Lipid content	Fraction	Normal	0.054 (SD = 0.0021)	0.0507
Moisture content	Fraction	Normal	0.71 (SD = 0.0033)	0.714
Dietary absorption efficiency of lipid	Fraction	Point estimate	0.92	0.92
Dietary absorption efficiency of NLOM	Fraction	Point estimate	0.60	0.60
Dietary absorption efficiency of water	Fraction	Point estimate	0.25	0.25
Fraction of porewater ventilated	Unitless	Point estimate	0	0
Northern Pikeminnow				
Weight	kg	Normal	0.558 (SD = 0.048)	0.599
Lipid content	Fraction	Normal	0.053 (SD = 0.008)	0.063
Moisture content	Fraction	Normal	0.719 (SD = 0.0088)	0.713
Dietary absorption efficiency of lipid	Fraction	Point estimate	0.92	0.92
Dietary absorption efficiency of NLOM	Fraction	Point estimate	0.60	0.60
Dietary absorption efficiency of water	Fraction	Point estimate	0.25	0.25
Fraction of porewater ventilated	Fraction	Point estimate	0	0

[a] Details of the parameters distribution selections are provided in Appendix ~~D~~B.

NLOM – non-lipid organic matter

SD – standard deviation

Table 5-11. Calibrated Values for Species-Specific Dietary Parameters

Species	Prey Item	Initial Distribution (%)[a]	Calibrated Value (%)
Zooplankton	Phytoplankton/algae	100	100
Benthic invertebrate filter feeders (clams)	Sediment solids	70 (50 – 80)	78
	Phytoplankton/algae	30 (20 – 50)	22
Benthic invertebrate consumers	Sediment solids	95 (85 – 100)	91
	Phytoplankton/algae	5 (0 – 15)	9
Epibenthic invertebrate consumers (crayfish)	Sediment solids	2 (0 – 4)	2
	Phytoplankton/algae	10 (0 – 20)	11
	Zooplankton	10 (0 – 20)	18
	Benthic invertebrates (filter feeders)	18 (0 – 35)	22
	Benthic invertebrates (consumers)	60 (25 – 75)	47

Table 5-11. Calibrated Values for Species-Specific Dietary Parameters

Species	Prey Item	Initial Distribution (%)[a]	Calibrated Value (%)
Sculpin	Sediment solids	0 (0 – 5)	3
	Zooplankton	0 (0 – 5)	3
	Benthic invertebrates (filter feeders)	15 (0 – 50)	32
	Benthic invertebrates (consumers)	80 (25 – 90)	53
	Epibenthic invertebrates (consumers)	5 (0 – 10)	9
Largescale sucker	Sediment solids	5 (1 – 15)	15
	Phytoplankton/algae	25 (0 – 60)	15
	Zooplankton	15 (5 – 25)	20
	Benthic invertebrates (filter feeders)	10 (5 – 15)	7
	Benthic invertebrates (consumers)	25 (15 – 35)	27
	Epibenthic invertebrates (consumers)	20 (0 – 40)	16
Common carp	Sediment solids	5 (0 – 10)	4
	Phytoplankton/algae	45 (30 – 60)	33
	Benthic invertebrates (filter feeders)	10 (5 – 15)	14
	Benthic invertebrates (consumers)	40 (25 – 55)	48
Smallmouth bass	Sediment solids	0	0
	Benthic invertebrates (consumers)	5 (0 – 30)	24
	Epibenthic invertebrates (consumers)	5 (0 – 30)	17
	Sculpin	90 (50 – 100)	59
Northern pikeminnow	Sediment solids	0	0
	Phytoplankton/algae	4 (0 – 10)	8
	Benthic invertebrates (filter feeders)	5 (0 – 10)	6
	Benthic invertebrates (consumers)	26 (15 – 45)	35
	Epibenthic invertebrates (consumers)	40 (25 – 65)	30
	Sculpin	25 (0 – 60)	21

[a] For all values in which a range is provided, a uniform distribution was assigned with the first number as the nominal value and the minimum and maximum defined by the range.

5.4.2 Calibration for Chemical-Specific Parameters

After calibration for non-chemical-specific parameters, the chemical concentration in water and the K_{OW} for each chemical were calibrated through probabilistic model runs using the calibrated non-chemical-specific parameters values as described in Section 5.2.5.3.2. When applicable, K_M~~metabolic rate constant~~s were then calibrated. During these model runs, the Study Area-wide sediment SWAC was used to represent the average sediment concentration. Table 5-12 provides the calibrated values for K_{OW} and water chemical concentration, and Table 5-13 presents the calibrated K_M~~metabolic rate constant~~s. Both tables present the initial distributions for these parameters for all chemicals for which the mechanistic model was used for PRG development.

Table 5-12. Chemical-Specific K_{OW} and Water Concentration

Chemical	K_{OW} Initial Distribution[a]	K_{OW} Calibrated Value	Water Concentration (ng/L) Initial Distribution[b]	Water Concentration (ng/L) Calibrated Value
PCBs				
Total PCBs[a]	6.09 – 7.84	6.14	0.217 (SD = 0.0244)	0.228
PCB 77	5.62 – 7.87	6.02	0.000261 (SD = 3.90×10^{-5})	0.000260
PCB 126	6.38 – 7.00	6.38	1.32×10^{-5} (SD = 1.04×10^{-6})	1.25×10^{-5}
~~**Dioxins and Furans**~~				
~~2,3,4,7,8-PeCDF~~	~~6.56 – 7.82~~	~~6.58~~	~~5.19×10^{-6} (SD = 5.97×10^{-7})~~	~~6.37×10^{-6}~~
Pesticides				
4,4′-DDD	4.82 – 6.33	5.83	0.049 (SD = 0.0090)	0.053
4,4′-DDE	4.28 – 6.97	6.42	0.031 (SD = 0.0028)	0.031
4,4′-DDT	3.98 – 8.31	6.31	0.017 (SD = 0.0021)	0.015
Aldrin	3.01 – 7.50	4.11	0.0022 (SD = 0.00022)	0.0023
alpha-HCH	3.19 – 4.57	4.08	0.027 (SD = 0.0040)	0.017
beta-HCH	3.19 – 4.26	3.43	0.0052 (SD = 0.00042)	0.0053
Dieldrin	2.60 – 6.20	5.26	0.067 (SD = 0.0092)	0.076
gamma-HCH	3.19 – 4.26	3.69	0.025 (SD = 0.0013)	0.028
Heptachlor	3.87 – 6.10	4.04	0.00021 (SD = 0.000016)	0.00019
Heptachlor epoxide	3.65 – 5.42	4.74	0.0071 (SD = 0.00044)	0.0072
Sum DDD	4.80 – 6.31	5.73	0.070 (SD = 0.013)	0.094
Sum DDE	4.22 – 6.87	6.45	0.032 (SD = 0.0029)	0.038
Sum DDT	3.98 – 8.19	6.00	0.022 (SD = 0.0024)	0.0217
Total chlordane	2.78 – 6.42	5.63	0.029 (SD = 0.0019)	0.031
Total DDx	4.34 – 7.08	5.91	0.13 (SD = 0.017)	0.139

[a] Uniform distributions developed from literature K_{OW} values were used to calibrate the model (see Appendix ~~D~~ B for additional information).

[b] Normal distributions based on XAD water samples from the Lower Willamette River were used to calibrate the model (see Appendix ~~D~~B for additional information).

DDD – dichlorodiphenyldichloroethane
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
HCH – hexachlorocyclohexane
K_{OW} – octanol-water partition coefficient
PCB – polychlorinated biphenyl
~~PeCDF – pentachlorodibenzofuran~~
SD – standard deviation
total DDx – sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE and 4,4′-DDT)

Table 5-13. Chemical-Specific Metabolic Rate Constants for Significantly Metabolized Chemicals

	Fish K_M (1/day)[a]			Invertebrate K_M (1/day)[b]		
Chemical	Nominal Value	Initial Distribution[c]	Calibrated Value	Nominal Value	Initial Distribution[c]	Calibrated Value
PCBs						
PCB 77	0.03	0 – 0.3	0.0070	NA	NA	NA
PCB 126	0.003	0 – 0.03	0.0064	NA	NA	NA
~~**Dioxins and Furans**~~						
~~2,3,4,7,8-PeCDF~~	~~0.03~~	~~0 – 0.3~~	~~0.024~~	~~0.03~~	~~0 – 0.3~~	~~0.095~~
Pesticides						
4,4′-DDT	0.01	0 – 0.1	0.010	0.01	0 – 0.1	0.058
Sum DDT	0.005	0 – 0.05	0.0078	NA	NA	NA

[a] The fish metabolic rate was applied equally to all modeled fish species (sculpin, largescale sucker, carp, smallmouth bass, and northern pikeminnow).

[b] ~~The invertebrate metabolic rate was applied to all invertebrate species for 2,3,4,7,8-PeCDF (benthic invertebrate filter feeders, benthic invertebrate consumers, and EICs).~~ For 4,4′-DDT, the metabolic rate was applied only to epibenthic invertebrate consumers.

[c] Uniform distributions were used to calibrate the model, as discussed in Appendix ~~D~~B.

DDT – dichlorodiphenyltrichloroethane
EIC – epibenthic invertebrate consumer
K_M – metabolic rate constant
NA – not applicable
PCB – polychlorinated biphenyl
~~PeCDF – pentachlorodibenzofuran~~

5.4.3 Calibrated Model Performance

After all non-chemical specific and chemical-specific model parameters were calibrated, model performance was evaluated both on a Study Area-wide basis and on smaller spatial scales for smallmouth bass and sculpin. The following subsections present this evaluation of model performance.

5.4.3.1 Study Area-Wide Spatial Scale

As described in Section 5.3.4, a SPAF was used to evaluate model performance. Table 5-14 shows the model performance for the calibrated model.

Table 5-14. Calibrated Model Performance

	SPAF[a]						
Chemical	Benthic Invertebrate Filter Feeder	Epibenthic Invertebrate Consumer	Sculpin	Largescale Sucker	Carp	Smallmouth Bass	Northern Pikeminnow
PCBs							
Total PCBs	4.5	**1.3**	2.0	1.4	3.7	**1.3**	**1.2**
PCB 77	2.3	1.1	**1.1**	ND	1.2	**1.1**	ND
PCB 126	1.1	**2.9**	**1.3**	ND	2.8	**1.4**	ND
~~**Dioxins and Furans**~~							

Table 5-14. Calibrated Model Performance

Chemical	SPAF[a]						
	Benthic Invertebrate Filter Feeder	**Epibenthic Invertebrate Consumer**	**Sculpin**	**Largescale Sucker**	**Carp**	**Smallmouth Bass**	**Northern Pikeminnow**
~~2,3,4,7,8-PeCDF~~	~~**(1.1)**~~	~~1.7~~	~~**(2.3)**~~	~~ND~~	~~1.0~~	~~1.6~~	~~ND~~
Pesticides							
4,4′-DDD	5.6	**(2.9)**	1.4	2.0	1.6	**(1.1)**	**(1.2)**
4,4′-DDE	4.7	**(1.4)**	1.6	2.5	2.4	**(1.2)**	2.7
4,4′-DDT	**(1.5)**	**(2.2)**	2.7	4.4	**(4.2)**	**(1.1)**	**(1.9)**
Aldrin	3.5	NE	6.0	NE	2.4[b]	**(1.5)**[b]	NE
alpha-HCH	**(1.2)**	NE	**(8.1)**[b]	NE	**(1.3)**[b]	**(1.1)**[b]	NE
beta-HCH	NE	NE	4.0[b]	NE	**(1.5)**[b]	**(1.2)**[b]	NE
Dieldrin	1.7	NE	3.9	NE	**(1.1)**	**(1.0)**[b]	NE
gamma-HCH	**(1.8)**	NE	3.2[b]	NE	**(1.3)**[b]	**(1.2)**[b]	NE
Heptachlor	1.2	NE	NE	NE	NE	**(1.2)**[b]	NE
Heptachlor epoxide	2.9	NE	3.6[b]	NE	**(1.1)**[b]	1.0[b]	NE
Sum DDD	5.8	**(3.1)**	1.4	2.0	1.8	**(1.0)**	**(1.1)**
Sum DDE	3.9	**(1.6)**	1.3	1.9	1.9	**(1.4)**	2.1
Sum DDT	1.0	**(3.1)**	3.4	3.8	**(2.7)**	**(1.1)**	**(1.0)**
Total chlordane	3.8	1.7[b]	2.4	NE	1.3	**(1.1)**	NE
Total DDx	3.4	**(1.7)**	2.1	1.9	1.2	**(1.2)**	1.6

[a] (**SPAFs)** shown in **bold** and in parentheses indicate that the model was over-predicting for this species-chemical combination.

[b] When high Round 1 reporting limits for non-detected chemical concentrations caused poor model performance, model results were compared to empirical data summarized without these non-detect data. See section 3.1.3 for a discussion of the analytical methods used for pesticides in Round 1 vs. Rounds 2 and 3 data.

DDD – dichlorodiphenyldichloroethane
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
HCH – hexachlorocyclohexane
ND – no data
NE – not evaluated (model performance not evaluated because there were five or fewer detected values)
PCB – polychlorinated biphenyl
~~PeCDF – pentachlorodibenzofuran~~
SPAF – species predictive accuracy factor
total DDx – sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE and 4,4′-DDT)

As discussed previously, model calibration emphasized model performance for smallmouth bass. All SPAFs for smallmouth bass are < 2, and SPAFs for other species are generally < 3. With four exceptions, all species-chemical combinations have SPAFs of < 5. These exceptions are discussed below:

- 4,4′-DDD for benthic invertebrate filter feeders – Model under-predicting by a large margin because of several high concentrations that inflate the Study Area-wide average.
- Sum DDD for benthic invertebrate filter feeders – Model under-predicting by a large margin because of several high concentrations that inflate the Study Area-wide average.
- Aldrin for sculpin – Model under-predicting by a factor of 6 because of high Round 1 reporting limits. Removing these 26 reporting limits from the dataset (of the 38 samples) causes the model to over-predict by a factor of 13. This indicates that the available data with detected concentrations (n=12) do not provide a comprehensive Study Area-wide dataset, and model performance should not be evaluated.
- Alpha-hexachlorocyclohexane (HCH) for sculpin – Model over-predicting by a factor of 8.1 when the 26 samples with high Round 1 reporting limits are removed. If these data are included, the model under-predicts by a factor of 7.6. The high over- and under-prediction of the sculpin data by the model indicates that this dataset does not represent the Study Area-wide average, and model performance should not be evaluated.

There is not a pattern of significant over- or under-prediction by species or chemical, indicating good overall model performance on a Study Area-wide basis.

5.4.3.2 Model Predictions Compared to Individual Sample Data

To further evaluate model performance, model-predicted tissue concentrations were graphed along with the full empirical tissue dataset for each species and the empirical mean and medians of the empirical data. Note that the following abbreviations are used in the graphs for ease of presentation:

- BIF – benthic invertebrate filter feeders (clams)
- BIC – benthic invertebrate consumers (worms)
- EIC – epibenthic invertebrate consumer (crayfish)
- SCL – sculpin
- LSS – largescale sucker
- CAR – carp
- SMB – smallmouth bass

- NPM – northern pikeminnow

Figures 5-2 through 5-16~~7~~ graphically display the results of calibrated model predictions compared to empirical data for the modeled chemicals. Field-collected empirical data are available for all species or species groups with the exception of benthic invertebrate consumers (only laboratory bioaccumulation test data are available for this species). Additionally, it should be noted that empirical data are not presented on the graphs for some chemical-species combinations because tissue was not analyzed for those combinations, or because the dataset available for this species was considered insufficient to represent Study Area-wide conditions.[17]

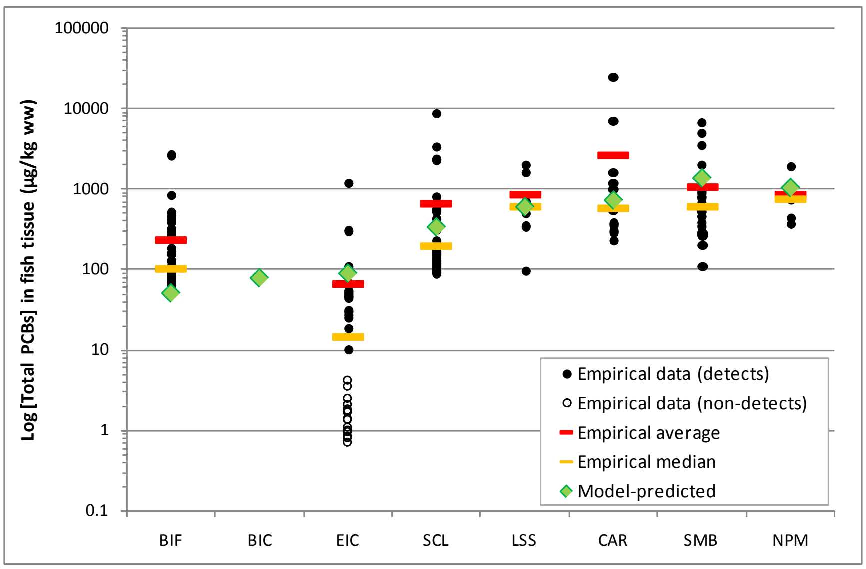


Figure 5-2. Empirical and Model-Predicted Data for Total PCBs

[17] Round 1 pesticide data for some species consisted of mostly high non-detect values. For datasets where these data significantly impacted Study Area-wide mean, the high Round 1 non-detect data were excluded from the dataset compared to mechanistic modeling predictions, as noted in Table 5-14.

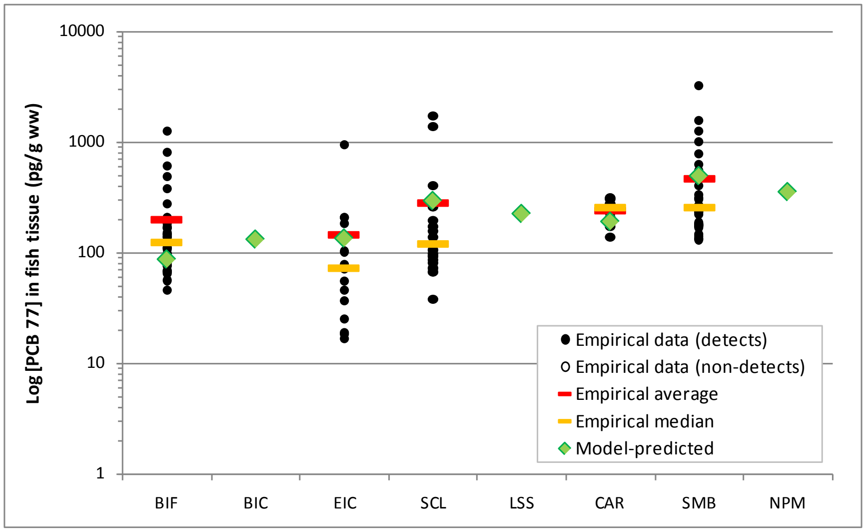


Figure 5-3. Empirical and Model-Predicted Data for PCB 77

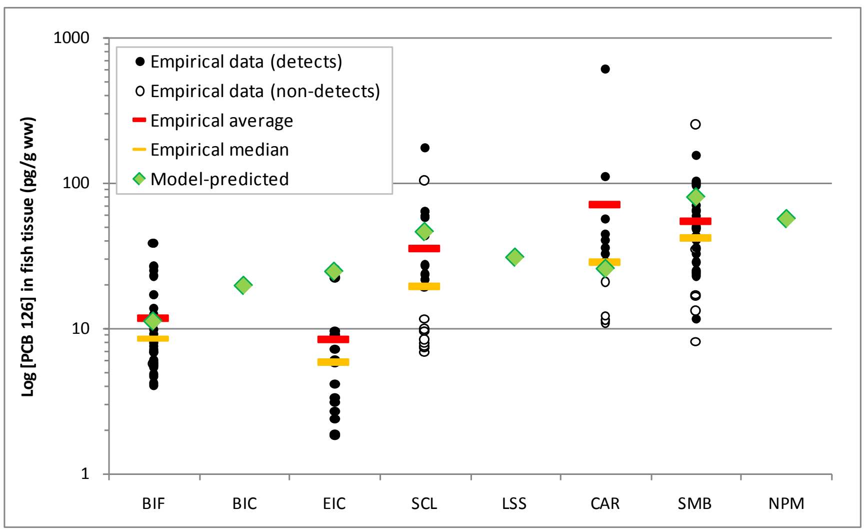
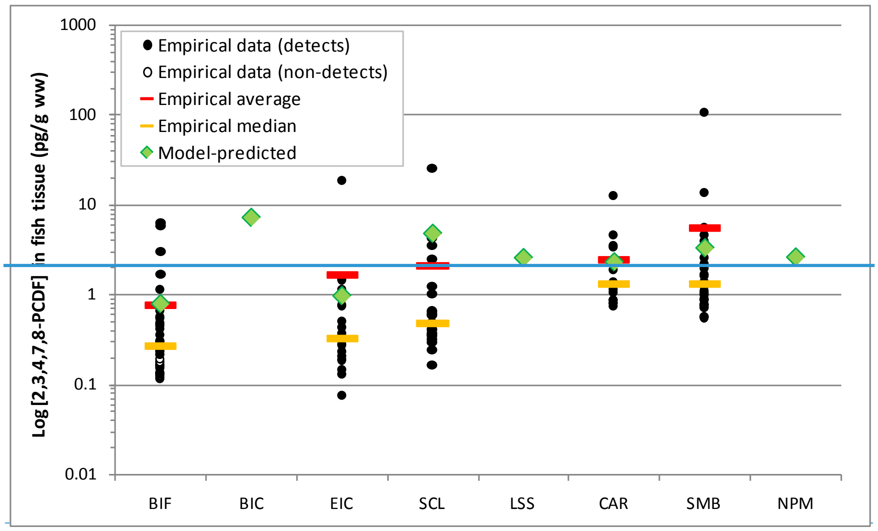


Figure 5-4. Empirical and Model-Predicted Data for PCB 126



~~**Figure 5-5. Empirical and Model-Predicted Data for 2,3,4,7,8-PeCDF**~~

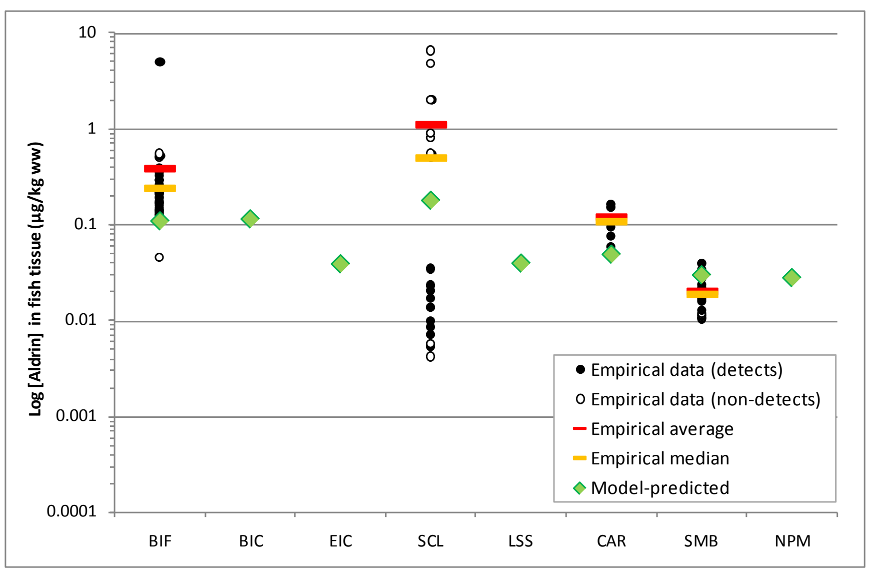


Figure 5-65. Empirical and Model-Predicted Data for Aldrin

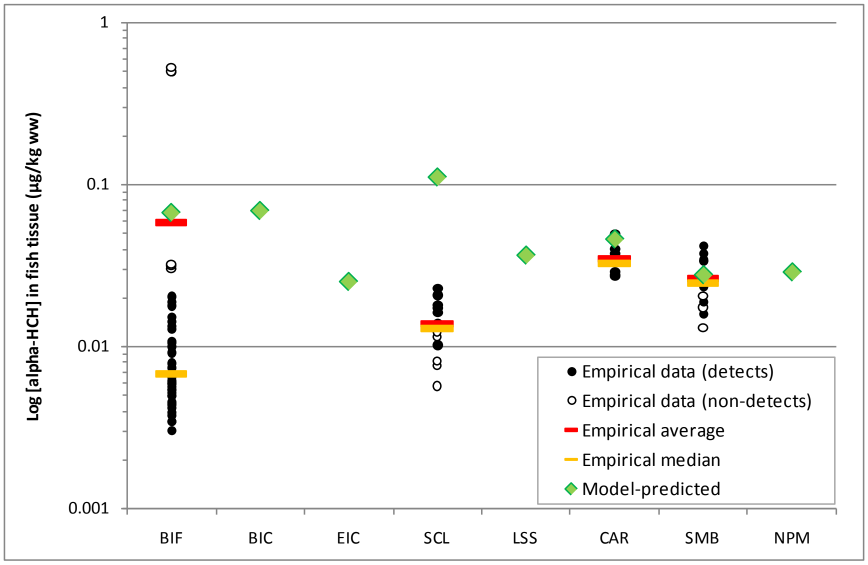


Figure 5-6~~7~~. Empirical and Model-Predicted Data for alpha-Hexachlorocyclohexane

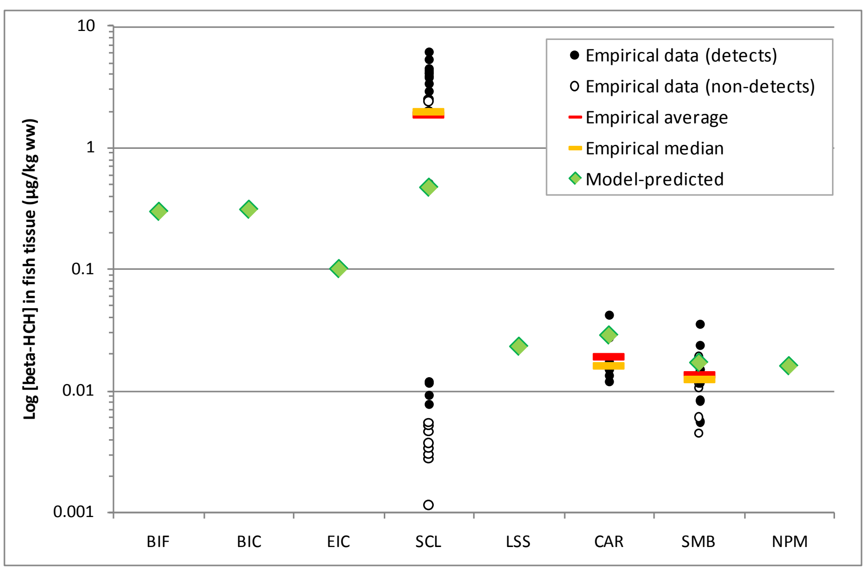


Figure 5-7~~8~~. Empirical and Model-Predicted Data for beta-Hexachlorocyclohexane

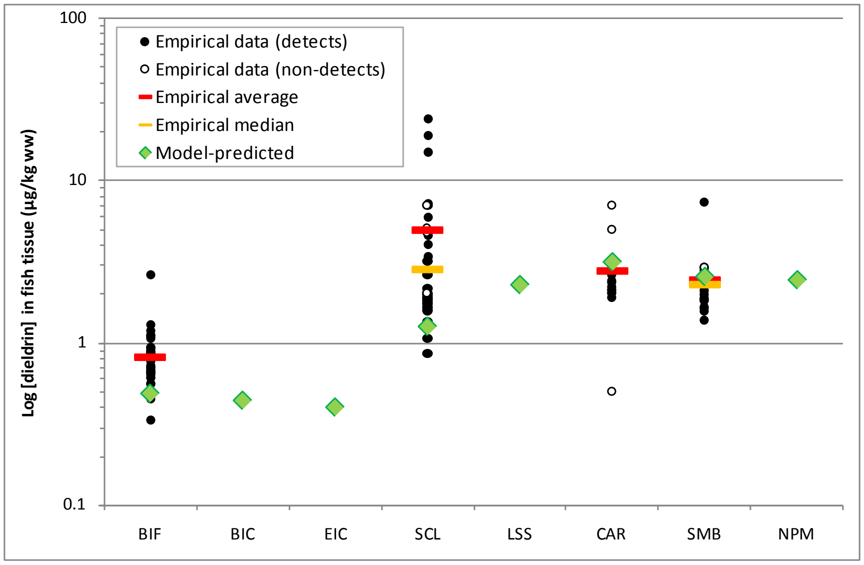


Figure 5-~~8~~9. Empirical and Model-Predicted Data for Dieldrin

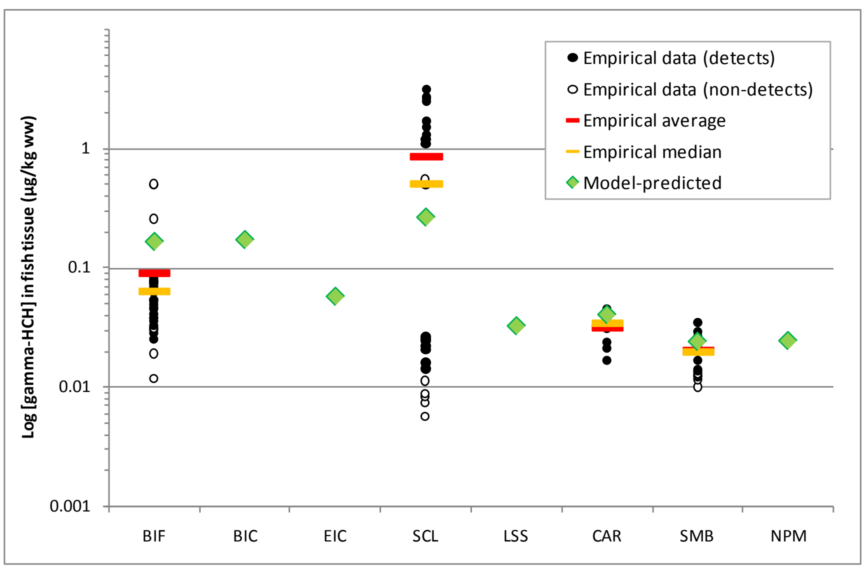


Figure 5-~~9~~10. Empirical and Model-Predicted Data for gamma-Hexachlorocyclohexane

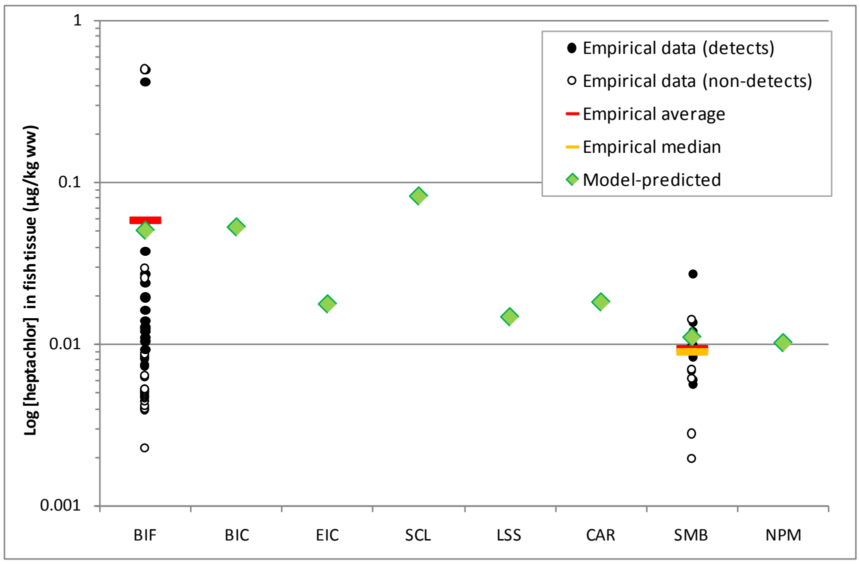


Figure 5-10~~1~~. Empirical and Model-Predicted Data for Heptachlor

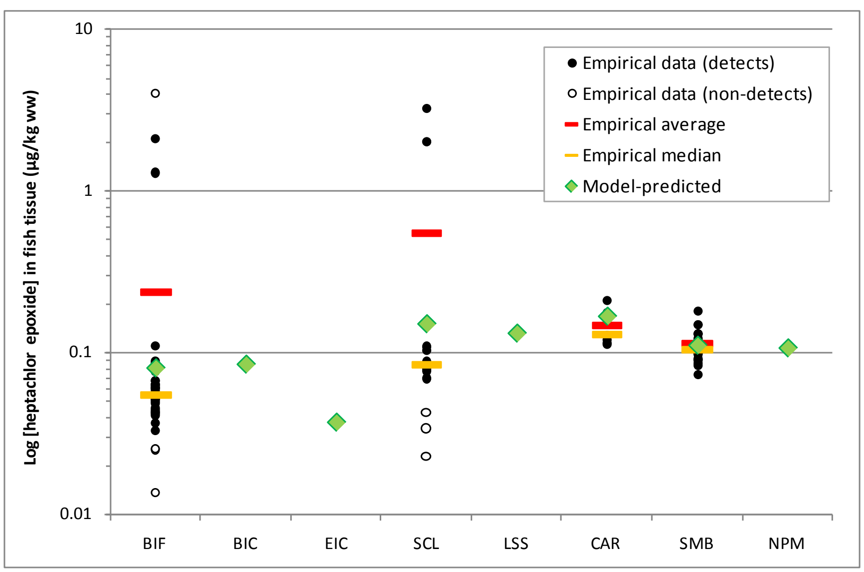


Figure 5-112. Empirical and Model-Predicted Data for Heptachlor Epoxide

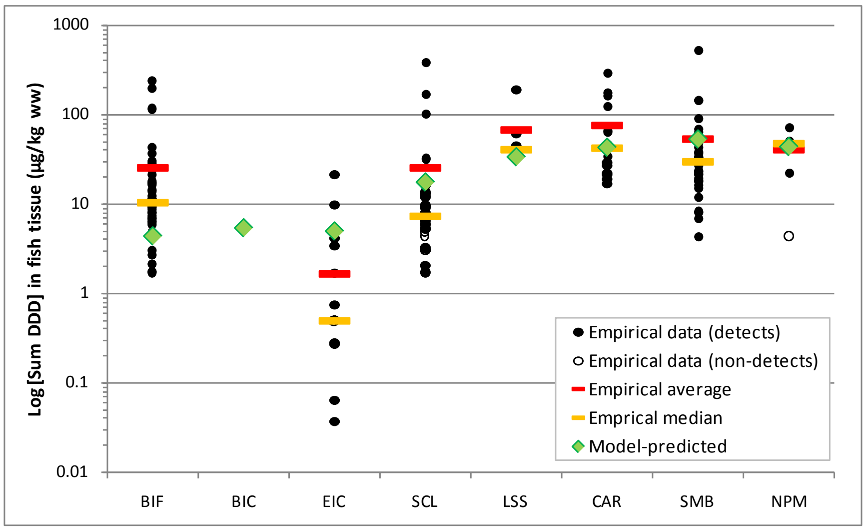


Figure 5-123. Empirical and Model-Predicted Data for Sum DDD

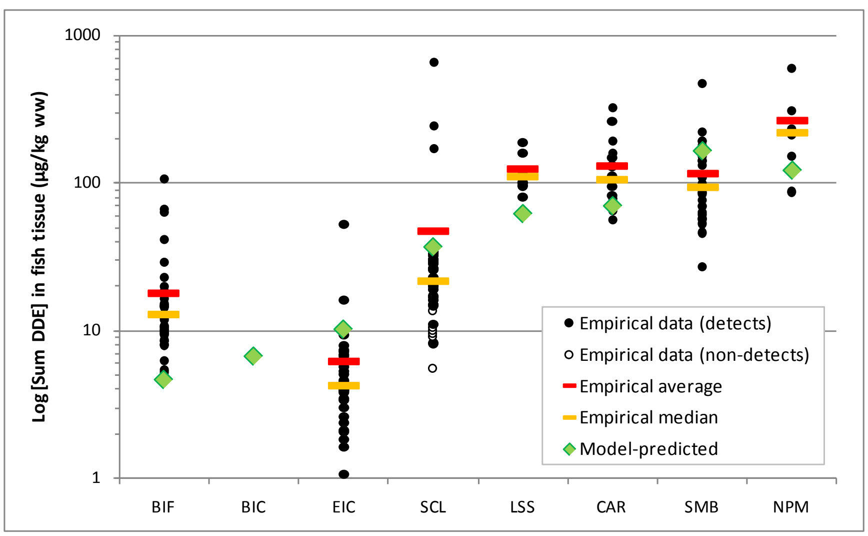


Figure 5-134. Empirical and Model-Predicted Data for Sum DDE

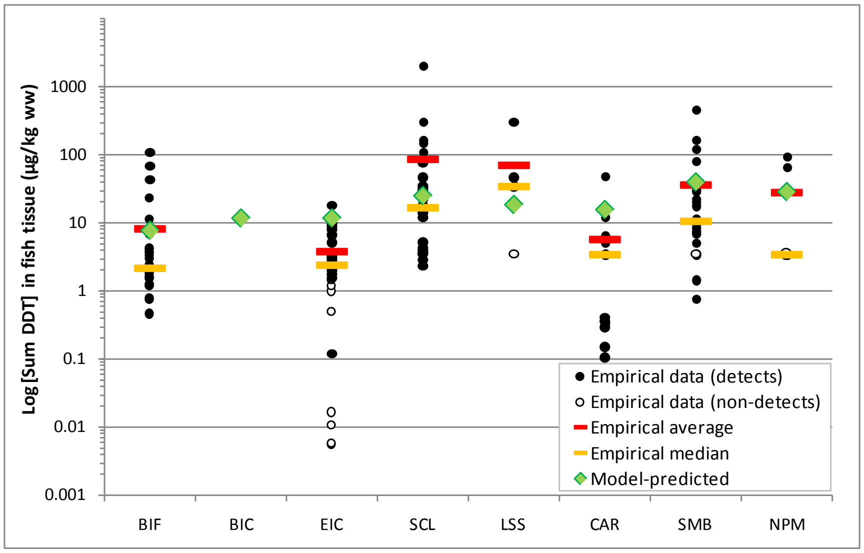


Figure 5-145. Empirical and Model-Predicted Data for Sum DDT

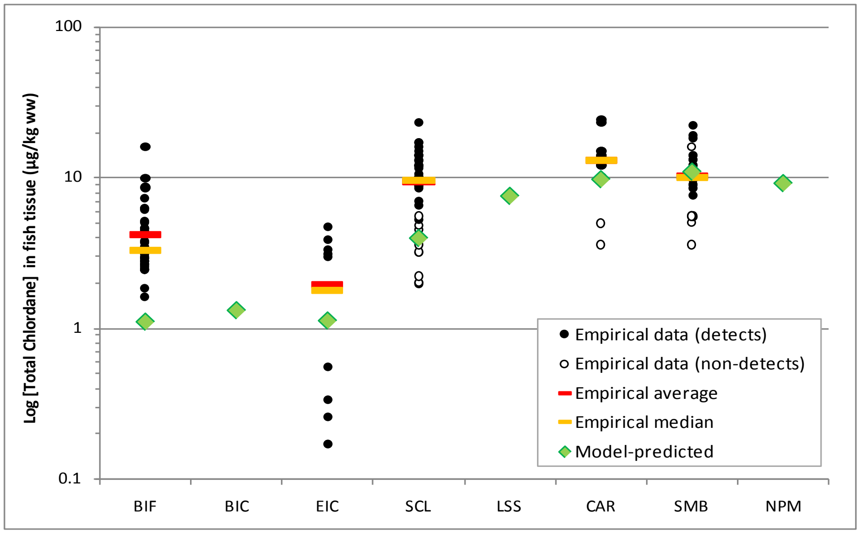


Figure 5-156. Empirical and Model-Predicted Data for Total Chlordane

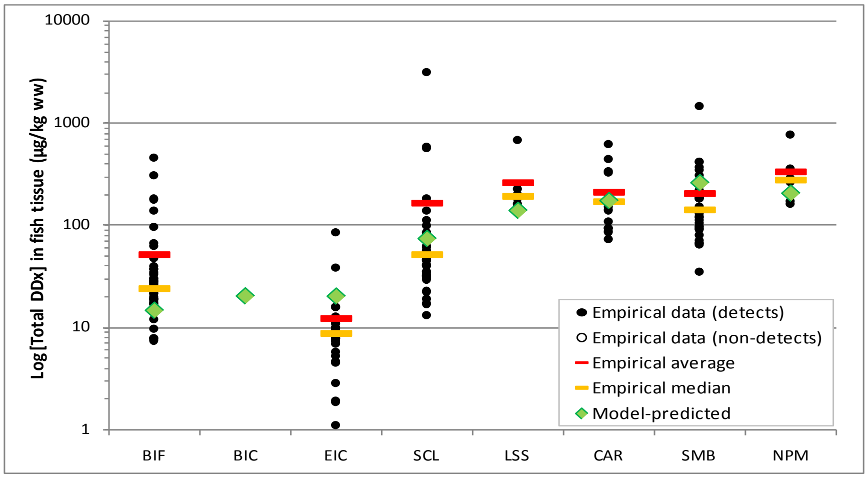


Figure 5-16~~7~~. Empirical and Model-Predicted Data for Total DDx

As indicated in Figures 5-2 to 5-16~~7~~, the majority of the model-predicted tissue concentrations (shown as green diamonds in the figures) are similar to the average empirical tissue concentration and are within the range of empirical data collected from the Lower Willamette River (indicated by the black dots on the figures, which show each individual empirical tissue data point).

5.4.3.3 Smaller Spatial Scale Model Application for Smallmouth Bass

The calibrated mechanistic model was also evaluated on smaller spatial scales for smallmouth bass. As described previously, smallmouth bass exposure areas were based on a 1-mile segment of the river (see Section 3.3.3). The mean SWAC for each composite was used in the model to predict the tissue concentration, and the minimum and maximum 1-mile SWACs were used to provide a range on the sediment concentration to which the smallmouth bass in the composite may have been exposed. In Swan Island Lagoon, no ranges of sediment exposure concentrations were available, and thus no error bars could be calculated for the bass composites. Because it is likely that bass and some of their prey leave the lagoon, they would be exposed to some degree to sediment concentrations similar to those experienced by the fish in RM 8 or RM 9. Figures 5-17~~8~~ to 5-23~~5~~ present model predictions and empirical data for individual bass composites by location for selected PCBs, dioxin/furans, and total DDx. Predicted and empirical tissue concentrations are on a wet-weight basis (see the y-axis on the left side of the graphs), while sediment concentrations are on a dry-weight basis (see the y-axis on the right side of the graphs). Both y-axes (for tissue and sediment) apply to empirical data and model predictions for the main stem of the river (RM 2 to RM 11) and Swan Island Lagoon (shown on the right side of the graphs).

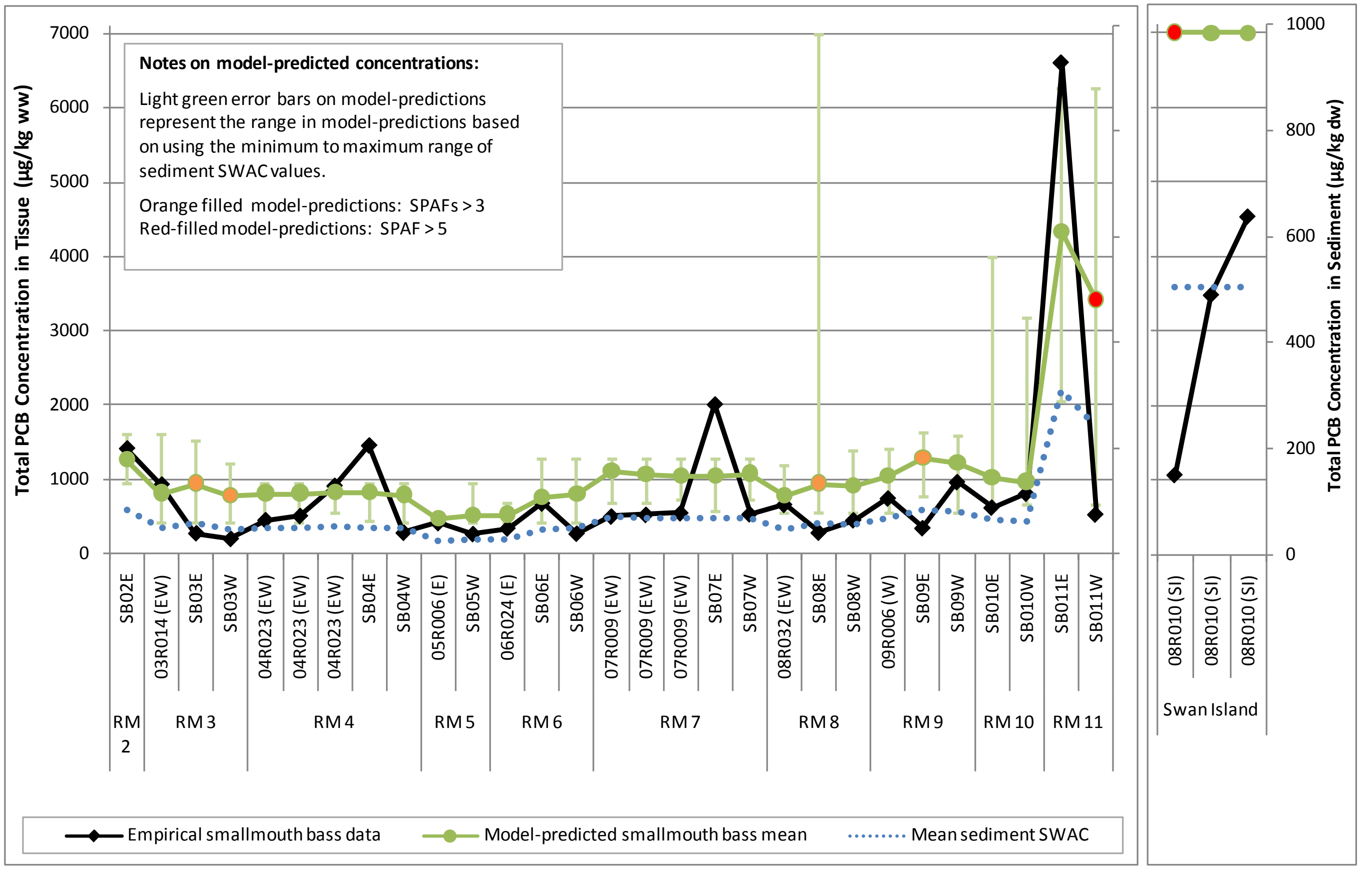


Figure 5-178. Empirical and Model-Predicted Smallmouth Bass Tissue Concentrations for Total PCBs for RM 2 through RM 11 and for Swan Island Lagoon

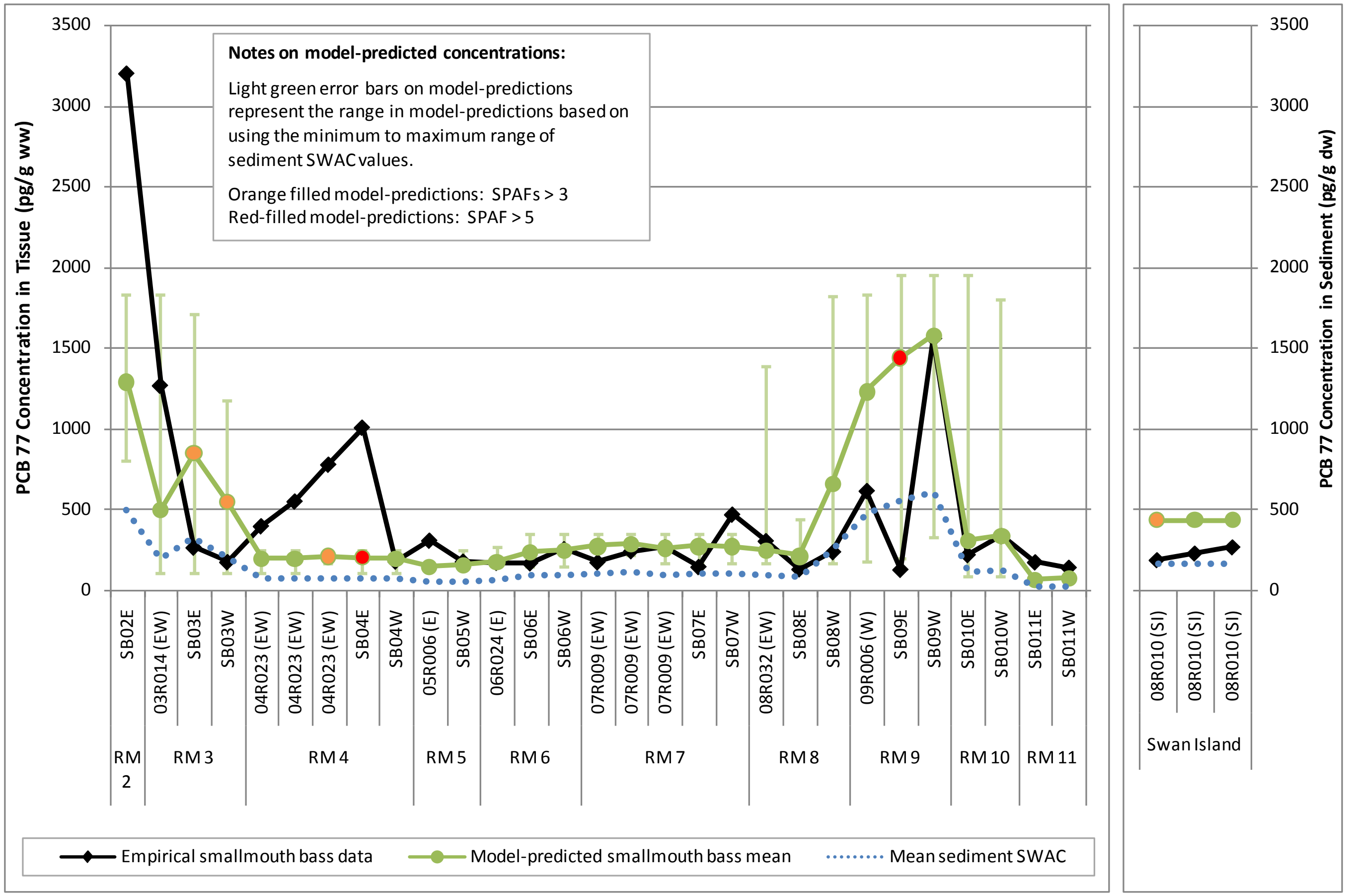


Figure 5-189. Empirical and Model-Predicted Smallmouth Bass Tissue Concentrations for PCB 77 for RM 2 through RM 11 and for Swan Island Lagoon

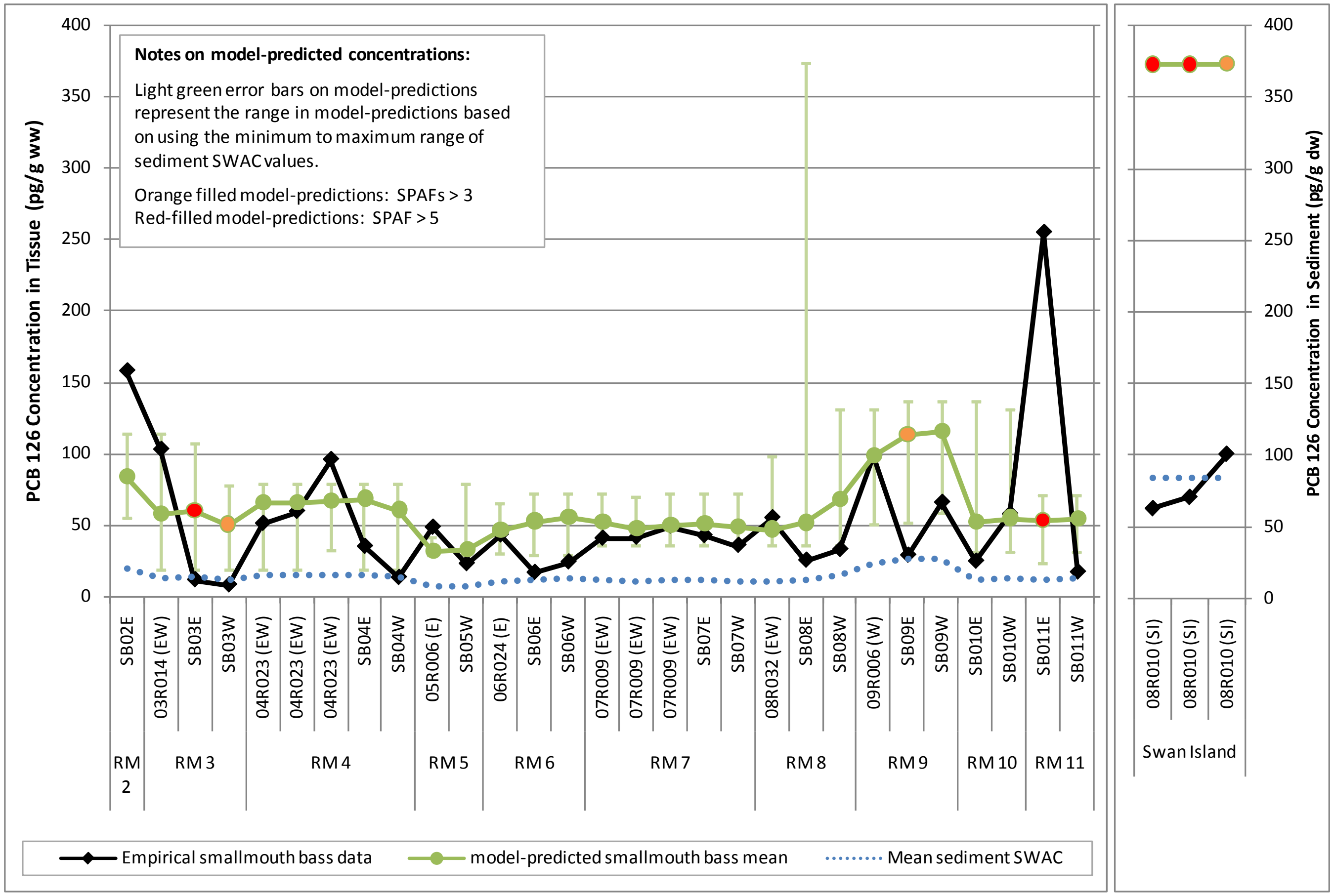
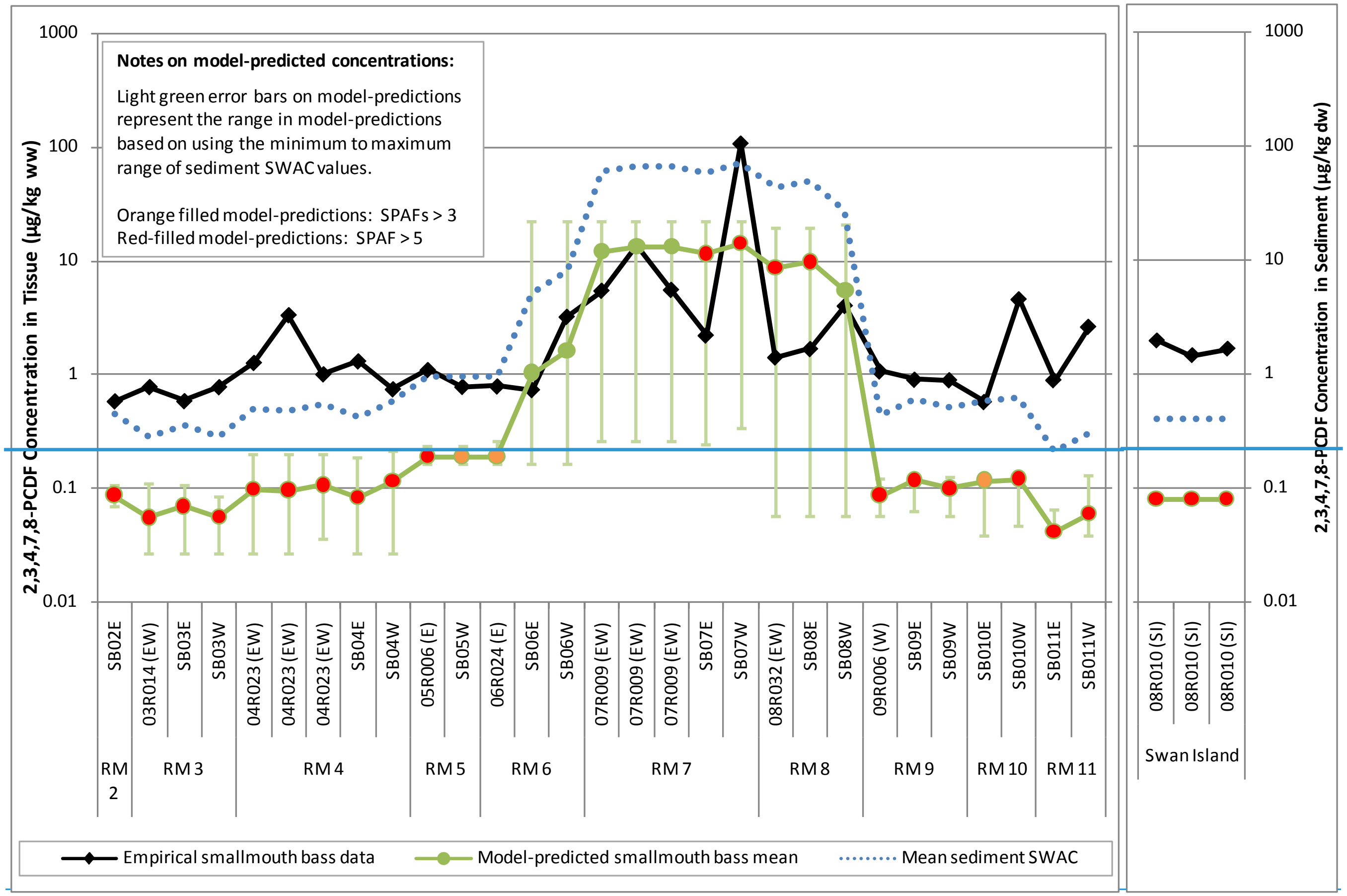


Figure 5-~~20~~19. Empirical and Model-Predicted Smallmouth Bass Tissue Concentrations for PCB 126 for RM 2 through RM 11 and for Swan Island Lagoon



~~**Figure 5-21. Empirical and Model-Predicted Smallmouth Bass Tissue Concentrations for 2,3,4,7,8-PeCDF for RM 2 through RM 11 and for Swan Island Lagoon**~~

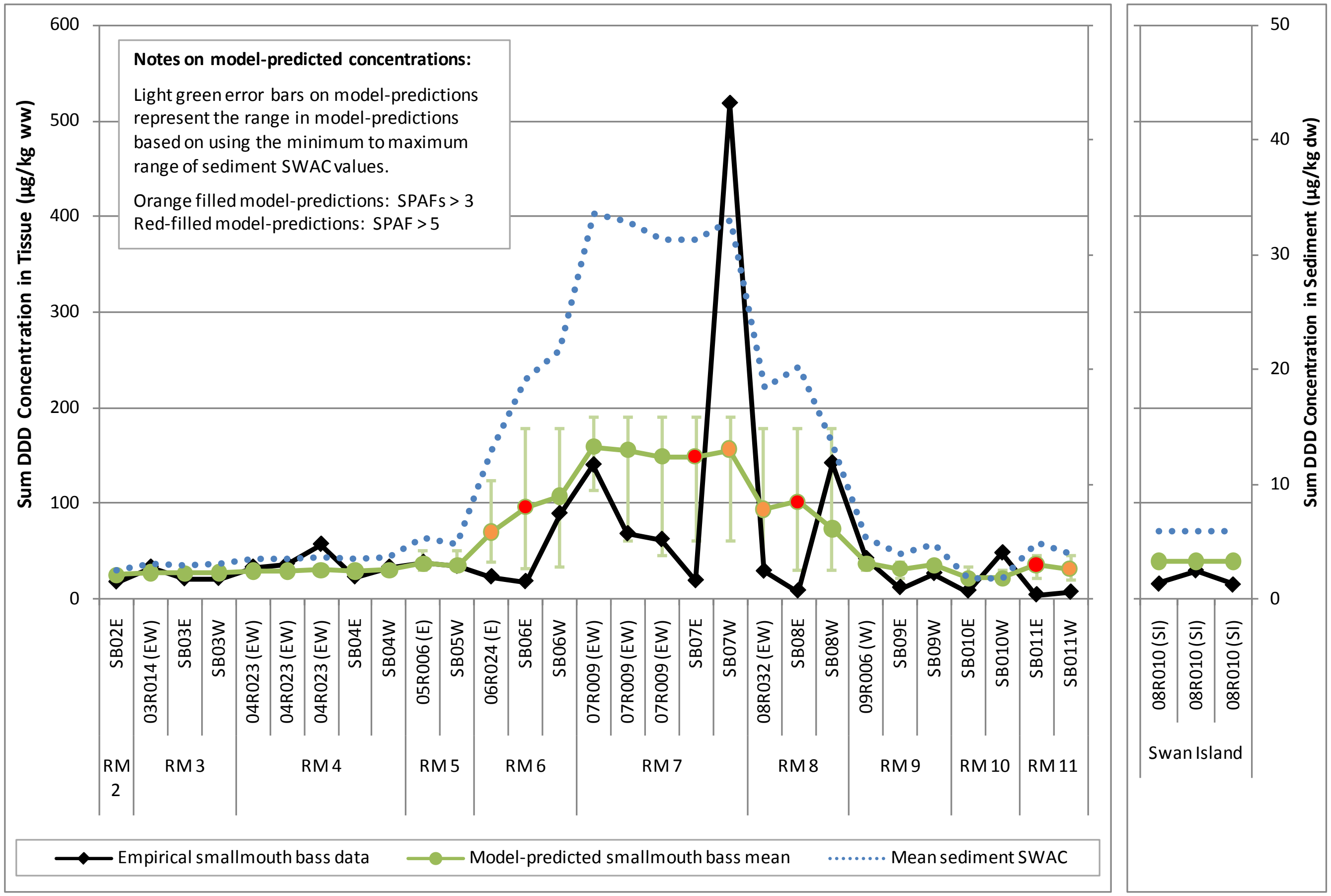


Figure 5-2~~0~~2. Empirical and Model-Predicted Smallmouth Bass Tissue Concentrations for Sum DDD for RM 2 through RM 11 and for Swan Island Lagoon

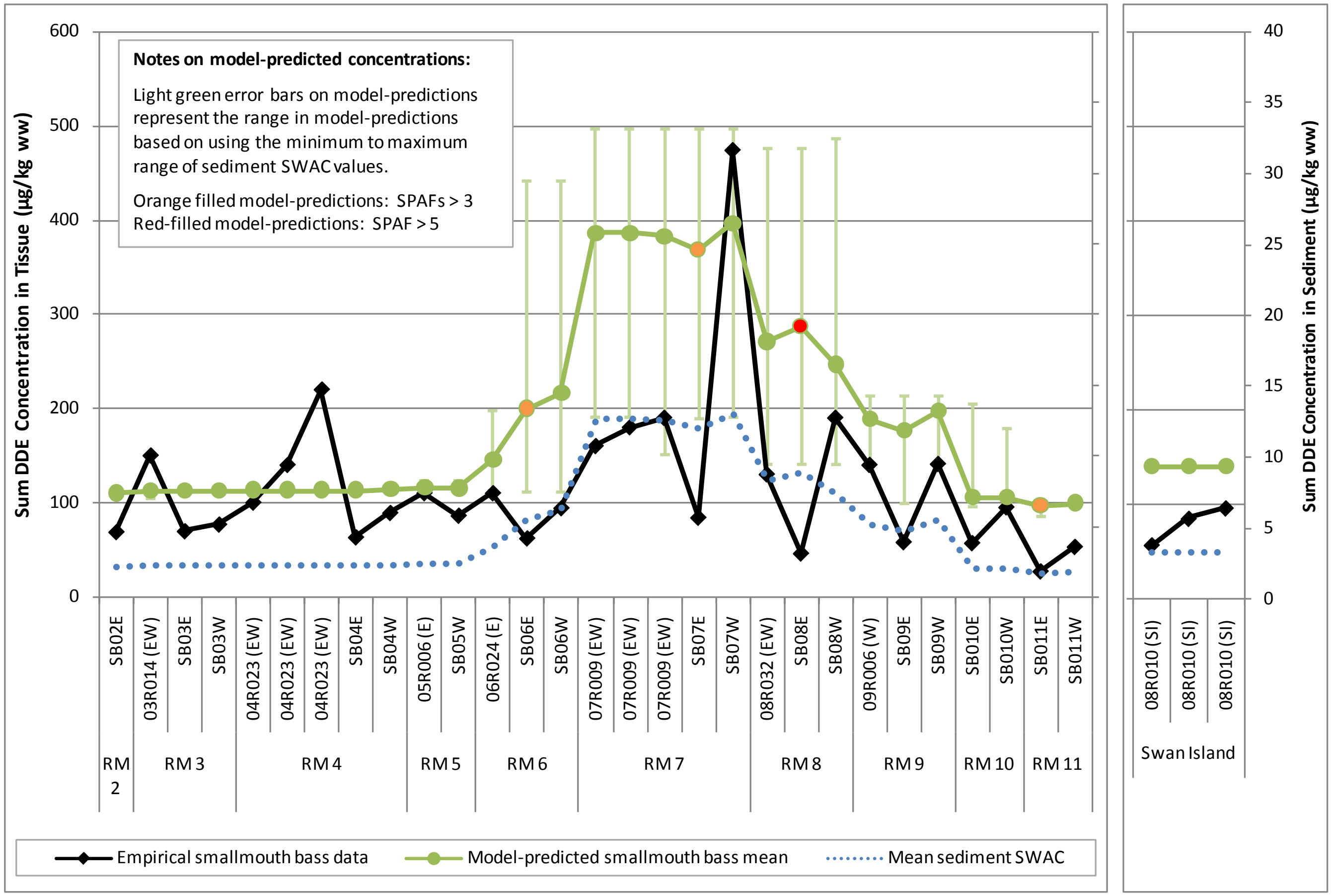


Figure 5-2~~13~~. Empirical and Model-Predicted Smallmouth Bass Tissue Concentrations for Sum DDE for RM 2 through RM 11 and for Swan Island Lagoon

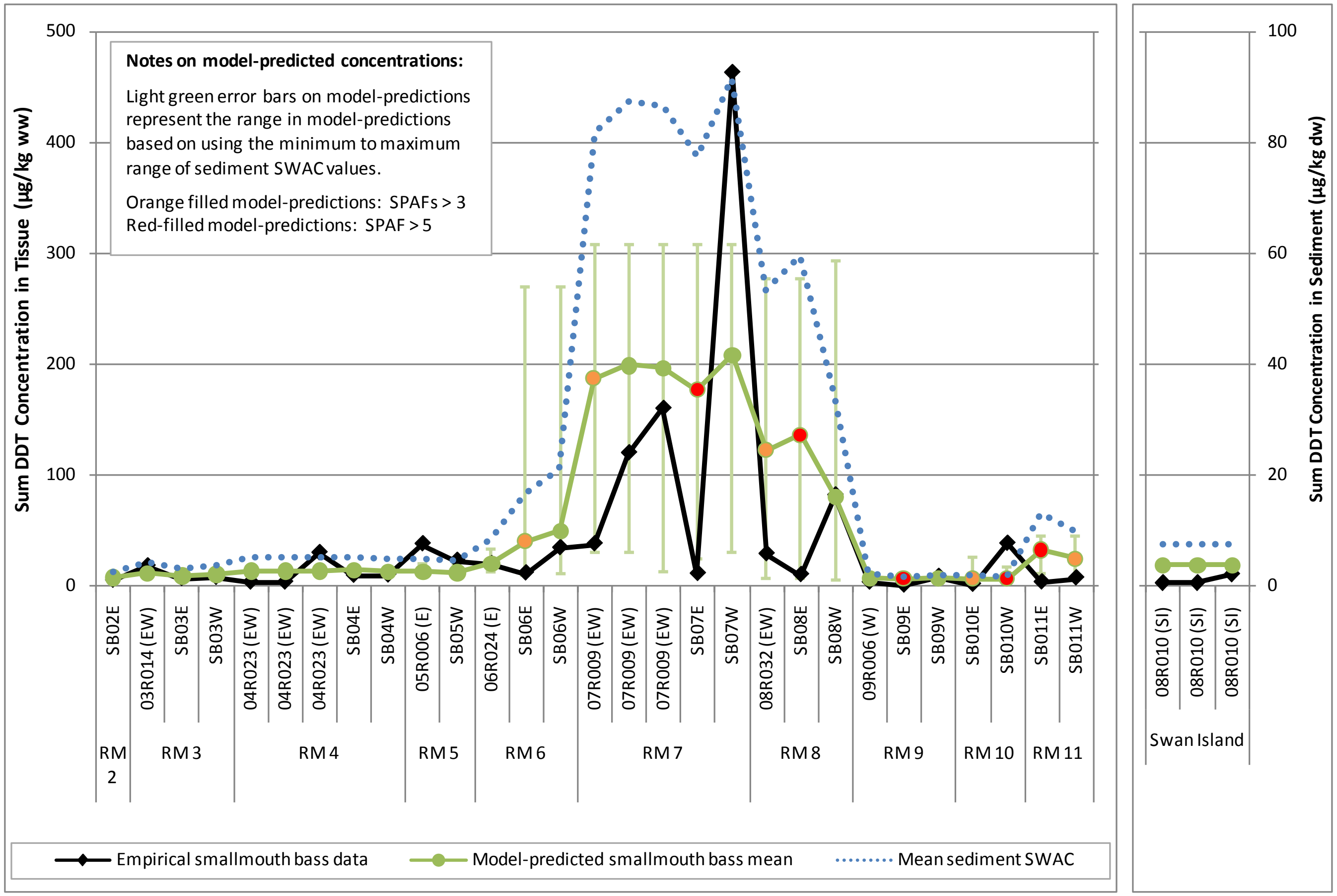


Figure 5-224. Empirical and Model-Predicted Smallmouth Bass Tissue Concentrations for Sum DDT for RM 2 through RM 11 and for Swan Island Lagoon

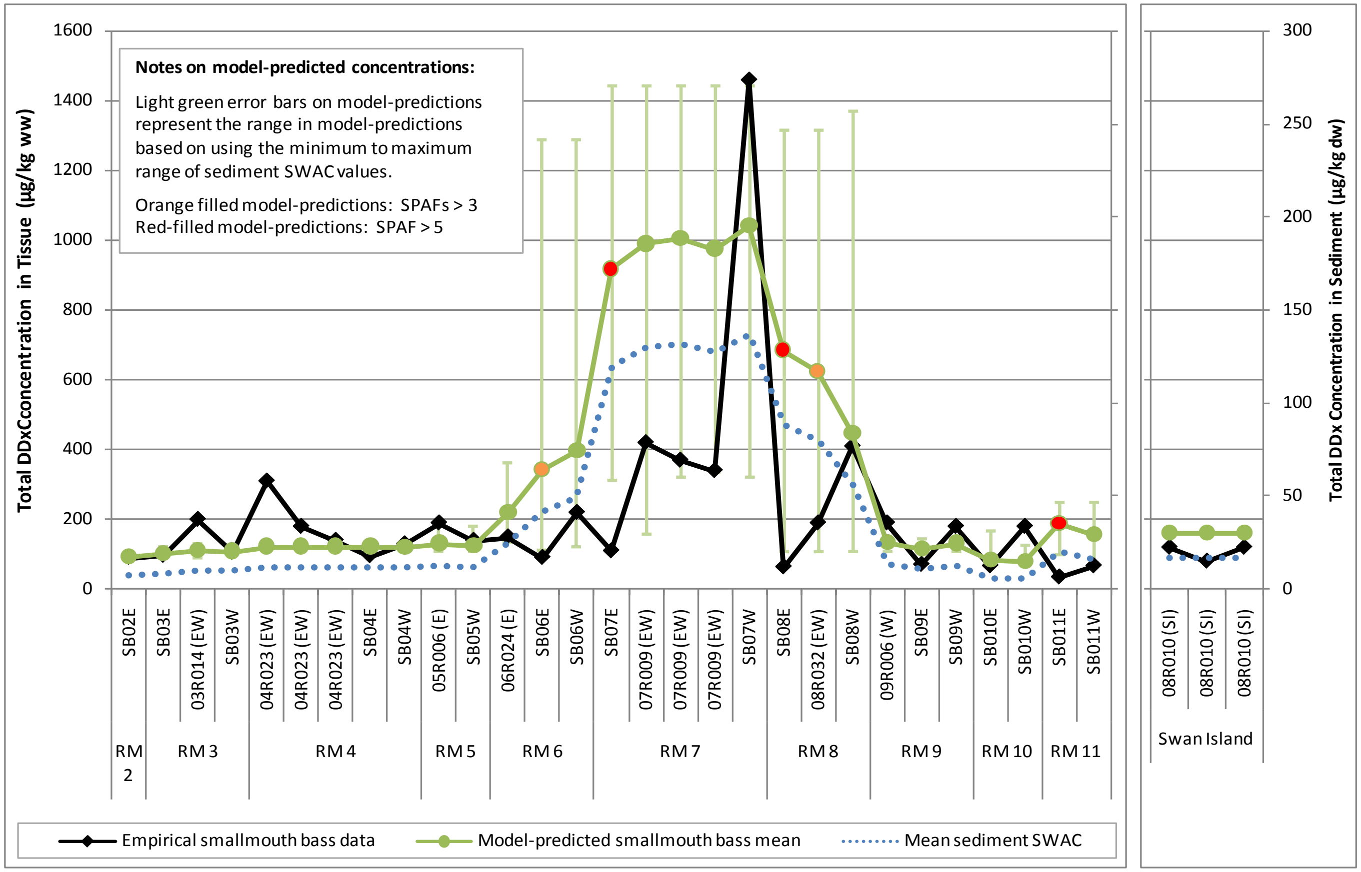


Figure 5-23~~5~~. Empirical and Model-Predicted Smallmouth Bass Tissue Concentrations for Total DDx for RM 2 through RM 11 and for Swan Island Lagoon

As can be seen in Figures 5-17~~8~~ to 5-23~~5~~, the mechanistic model generally predicts the empirical data within a factor of 3 based on the mean SWAC for each composite. Locations where the model does not predict as well based on the mean sediment SWAC are generally areas with high variability in the sediment and thus a high level of uncertainty in the sediment concentration to which the bass in a given composite were exposed. The uncertainty about these model predictions are represented by error bars calculated based on the minimum and maximum 1-RM SWACs that could be applicable to a given bass composite (see Section 3.3.3 for more details). These error bars generally overlap the empirical data for the smallmouth bass composite samples, further indicating that the model is predicting well on a smaller spatial scale.

For the purposes of this assessment, it was assumed that smallmouth bass collected inside of Swan Island Lagoon and their prey do not leave this area. Only one sediment SWAC was calculated for this area, and thus no range of sediment concentrations is available to bound the uncertainty surrounding the sediment concentration to which the bass are exposed (i.e., no error bars could be calculated). This uncertainty is less important for DDDs, DDEs, and DDTs (Figures 5-20~~2~~ to 5-23~~5~~) where the model predicts well based on the Swan Island Lagoon SWAC, likely because sediment concentrations on the east side of RM 8 and RM 9 are similar to those in Swan Island Lagoon for these chemicals.

However, for PCBs~~ and dioxins/furans~~, there is generally much higher variability in the sediment concentrations found in Swan Island Lagoon and on the east side of RM 8 and RM 9. For PCBs, the model over-predicts the bass tissue concentrations in Swan Island Lagoon, perhaps because the bass collected from Swan Island Lagoon (where sediment concentrations are higher) and their prey were also exposed to the lower sediment concentration in RM 8 and RM 9 (Figures 5-17~~8~~ to 5-19~~20~~). ~~For 2,3,4,7,8-PeCDF, the situation is reversed (the model underpredicts the bass tissue concentrations in Swan Island Lagoon), which is consistent because the 2,3,4,7,8-PeCDF sediment concentration is lower in Swan Island Lagoon than in RM 8 and RM 9 (Figure 5-21).~~

5.4.3.4 Smaller Spatial Scale Model Application for Sculpin

The calibrated mechanistic model was also evaluated on smaller spatial scales for sculpin. As described previously, sculpin exposure areas were based on a circle with a radius of 0.1 mile (see Section 3.3.3). Similar to the procedure for smallmouth bass, the SWAC for the 0.1-mile-radius circle was used in used in the model to predict individual sculpin composite tissue concentrations, and the minimum and maximum sediment concentrations within that circle were used to generate predictions assuming a range on the sediment concentrations to which the sculpin in the composite may have been exposed. Figures 5-24~~6~~ to 5-30~~3~~ show model prediction and empirical data for individual sculpin composites by location for selected PCBs, dioxin/furans, and total DDX. Tissue concentrations are on a wet-weight basis and sediment concentrations are on a dry-weight basis.

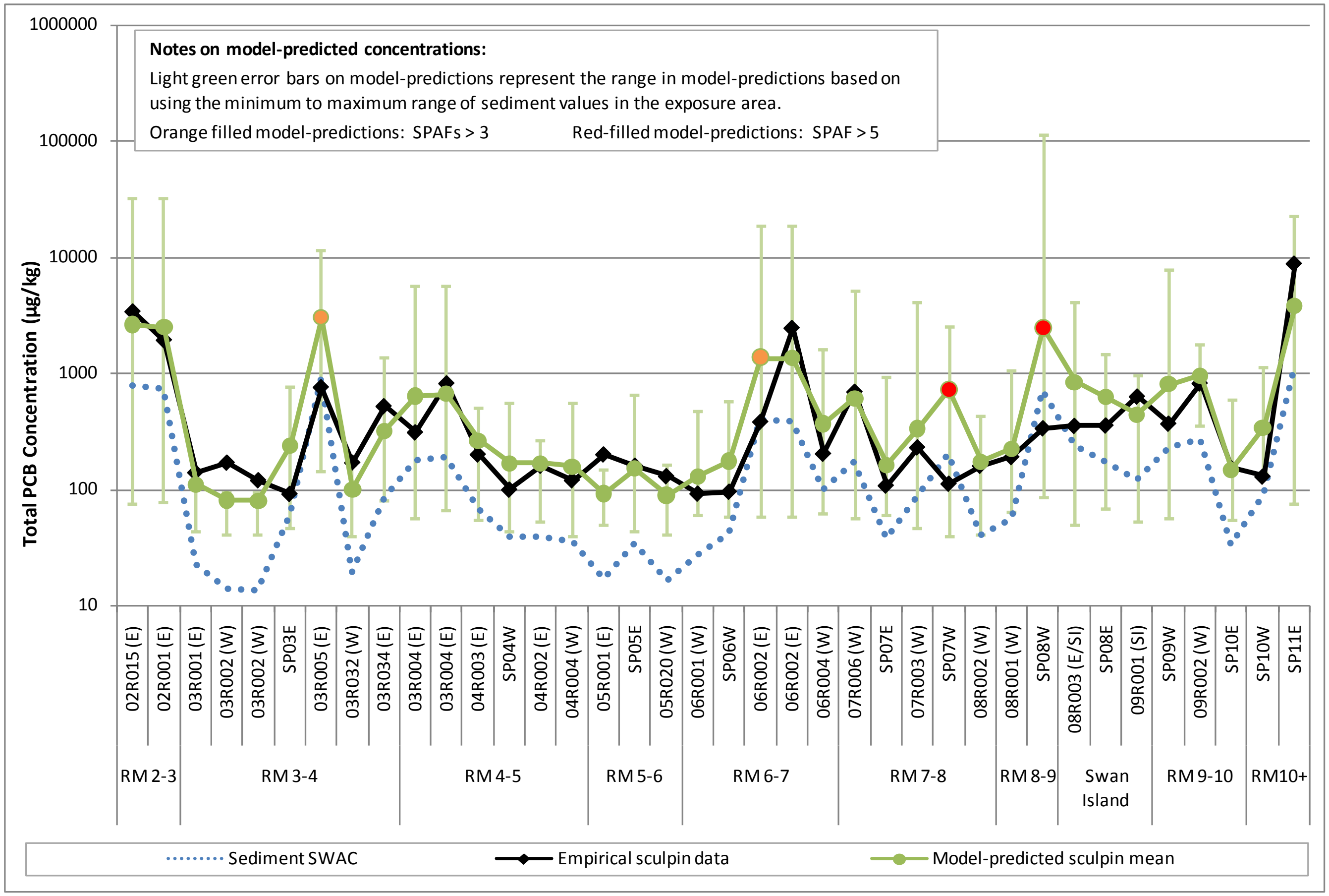


Figure 5-2~~4~~6. Empirical and Model-Predicted Sculpin Tissue Concentrations for Total PCBs for RM 2 through RM 11

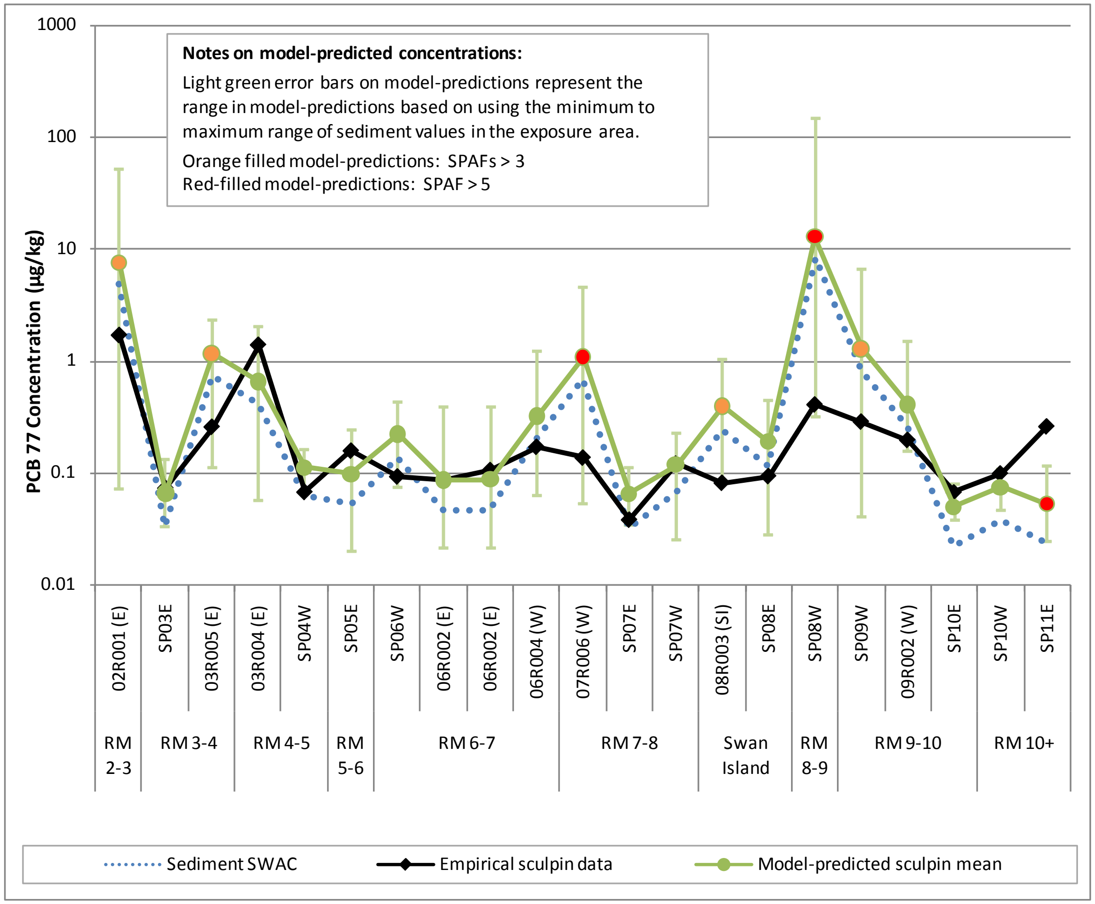


Figure 5-2~~57~~. Empirical and Model-Predicted Sculpin Tissue Concentrations for PCB 77 for RM 2 through RM 11

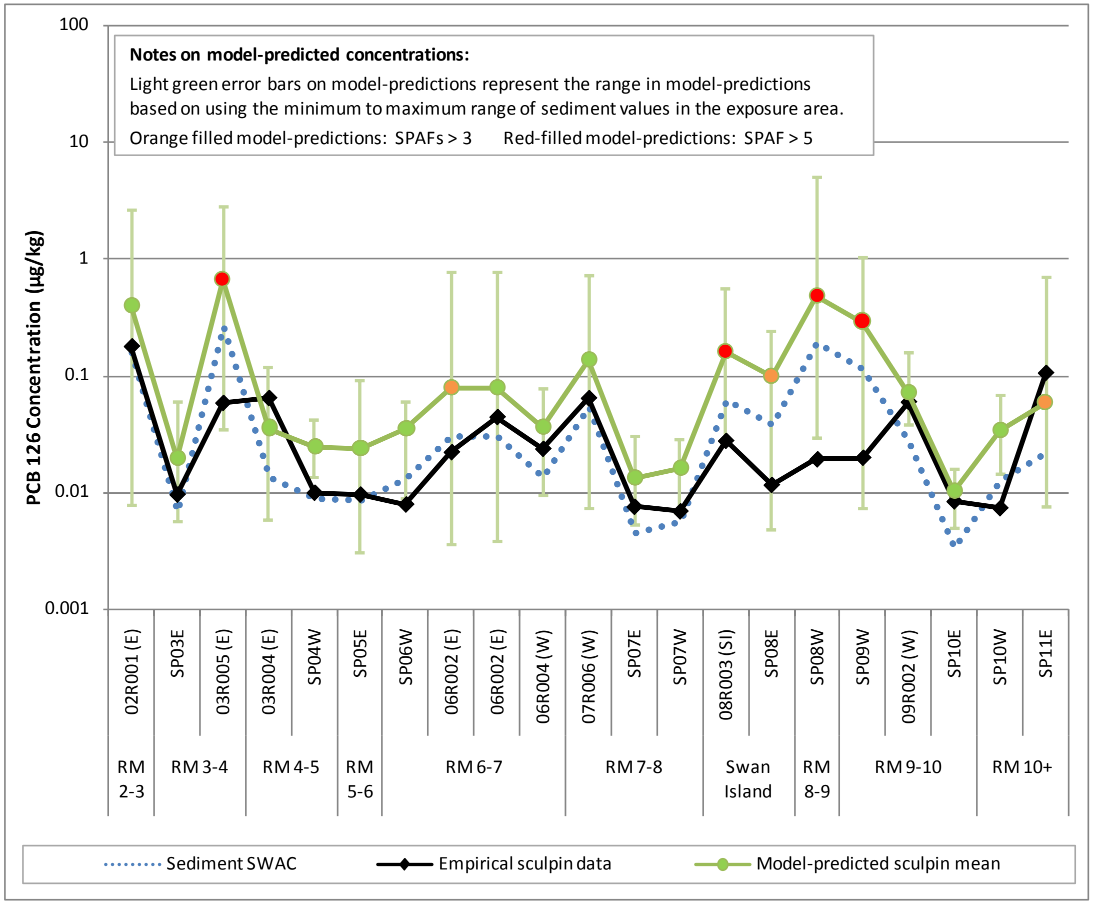
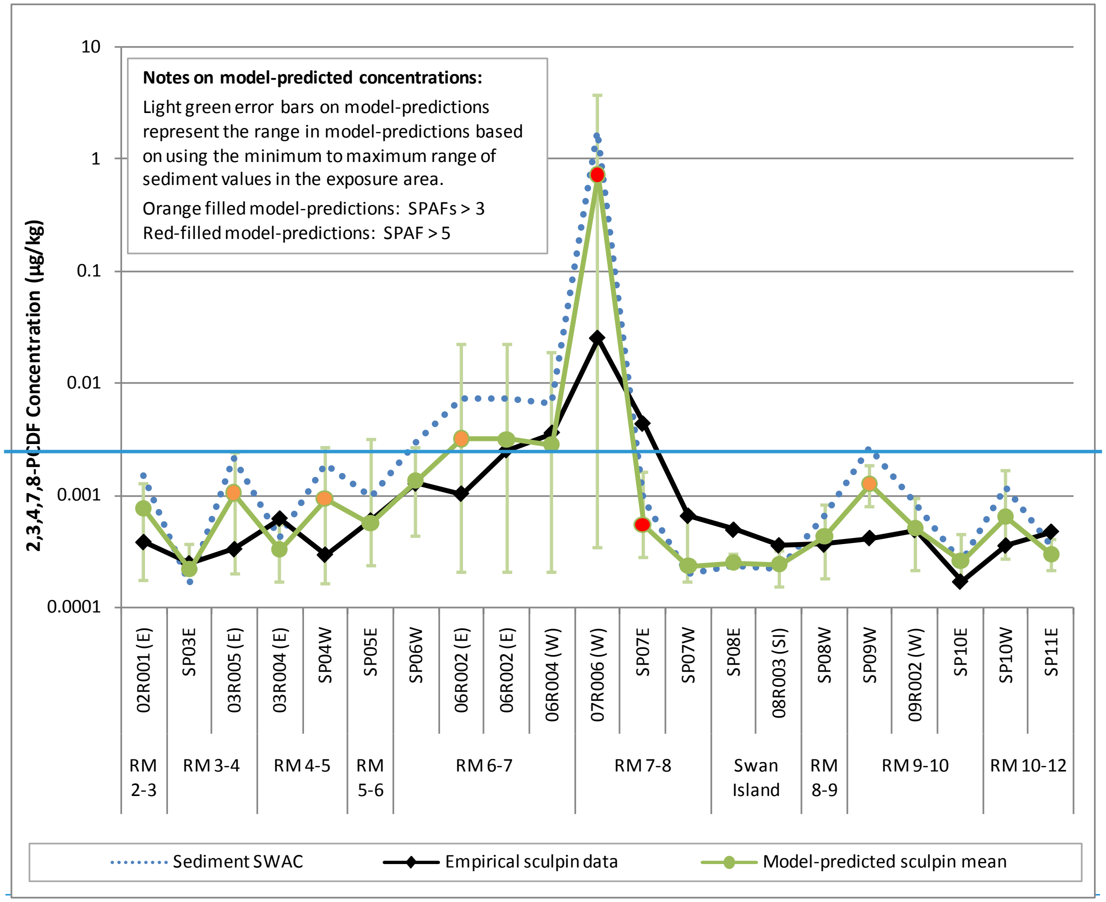


Figure 5-2~~6~~8. Empirical and Model-Predicted Sculpin Tissue Concentrations for PCB 126 for RM 2 through RM 11



~~**Figure 5-29. Empirical and Model-Predicted Sculpin Tissue Concentrations for 2,3,7,8-PeCDF for RM 2 through RM 11**~~

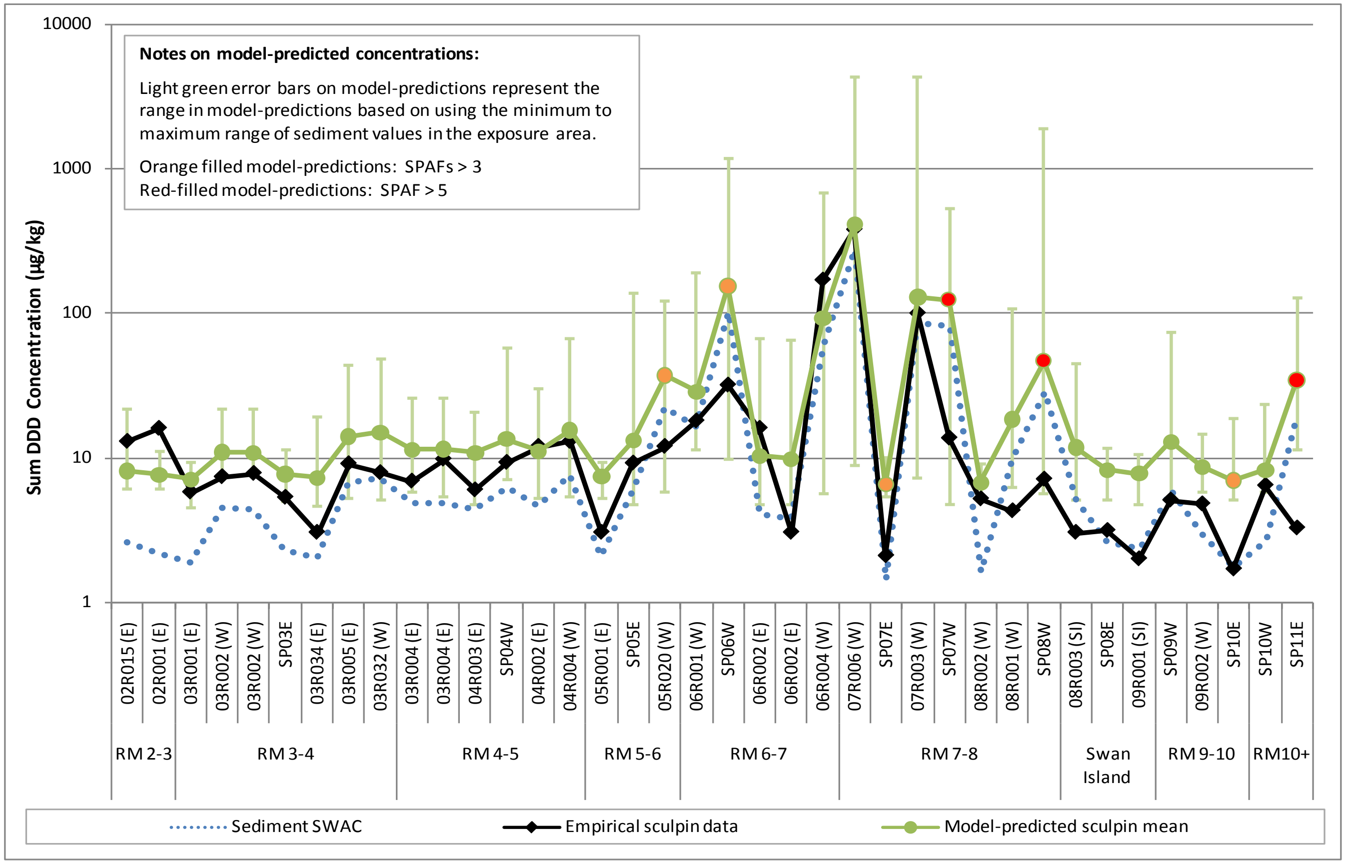


Figure 5-~~30~~27. Empirical and Model-Predicted Sculpin Tissue Concentrations for Sum DDD for RM 2 through RM 11

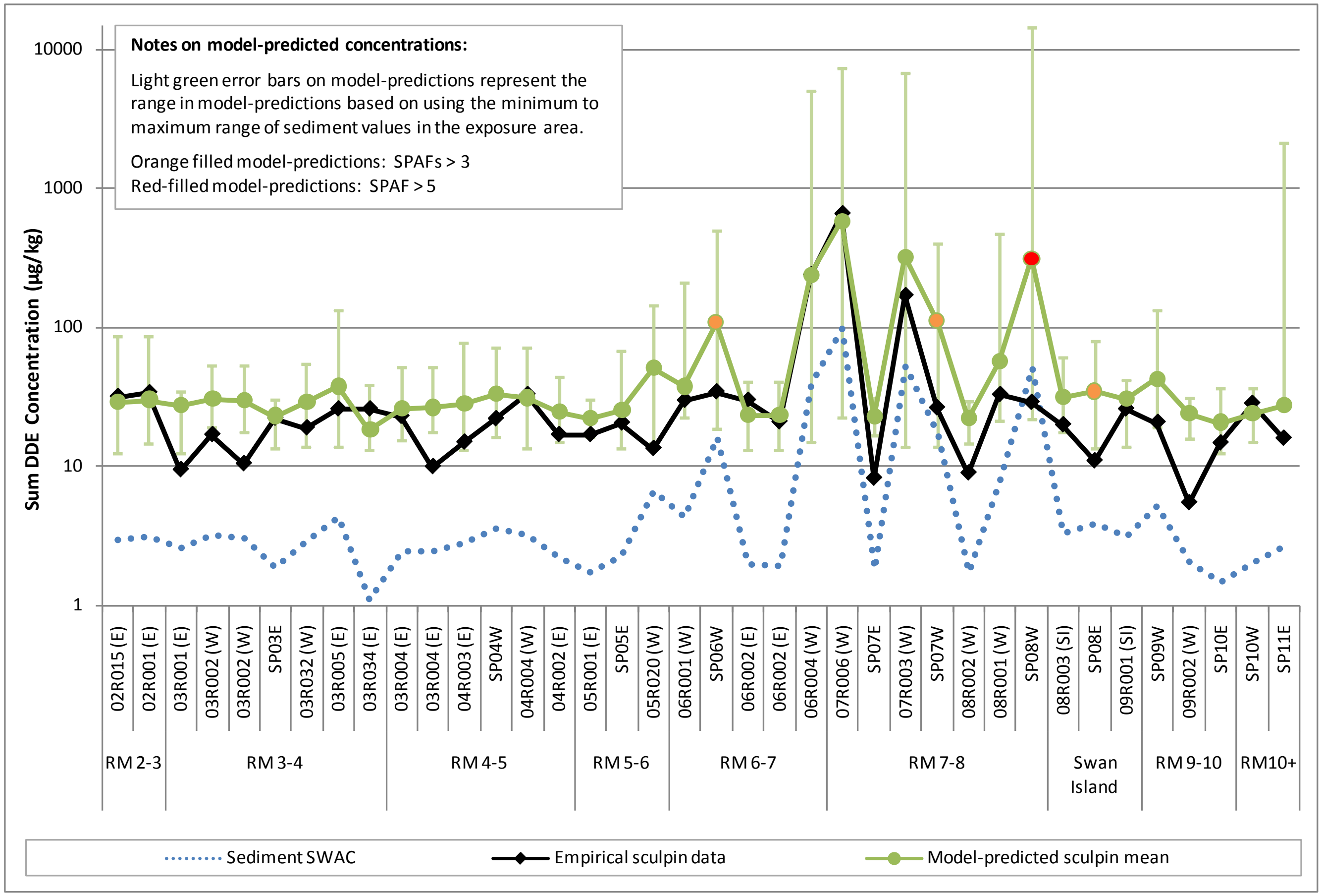


Figure 5-~~31~~28. Empirical and Model-Predicted Sculpin Tissue Concentrations for Sum DDE for RM 2 through RM 11

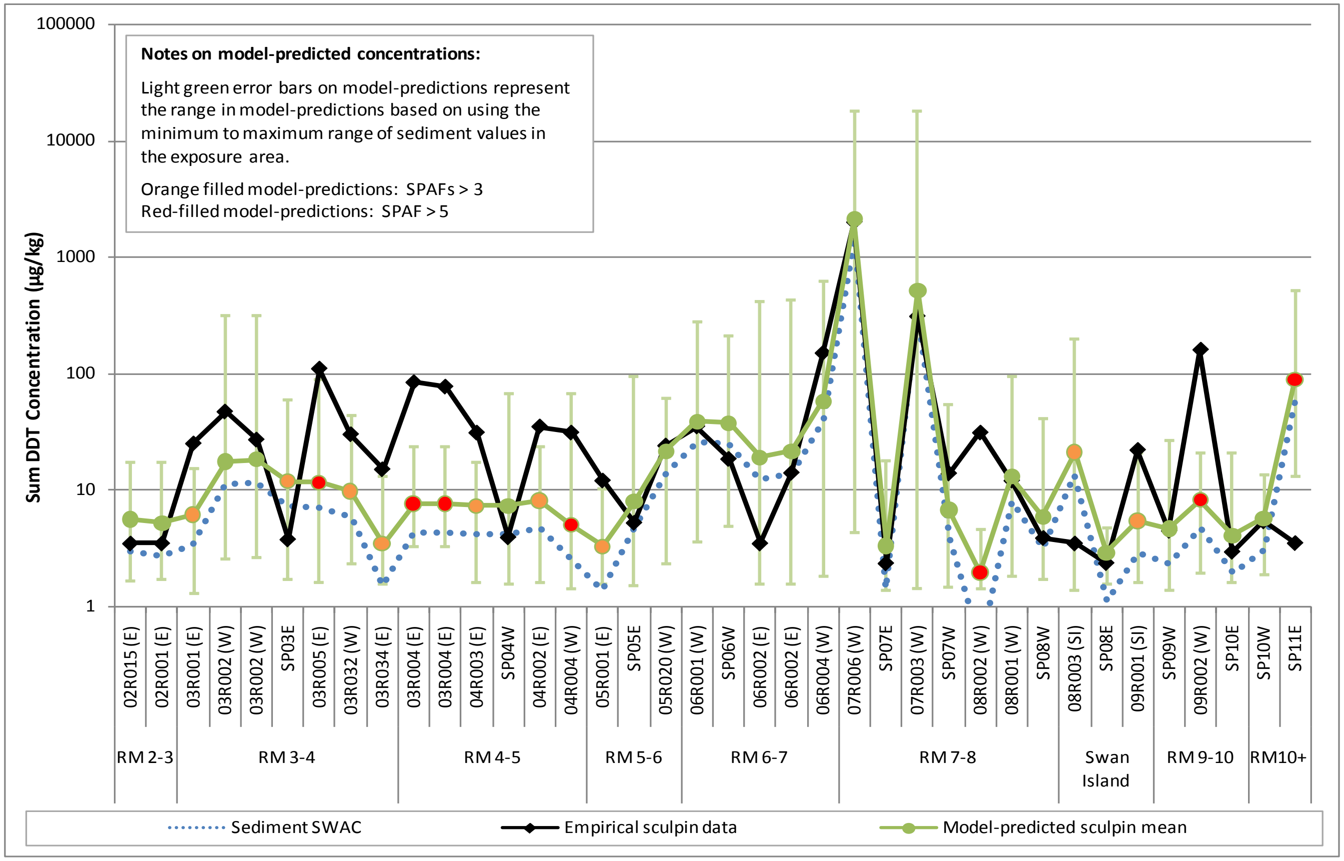


Figure 5-~~32~~29. Empirical and Model-Predicted Sculpin Tissue Concentrations for Sum DDT for RM 2 through RM 11

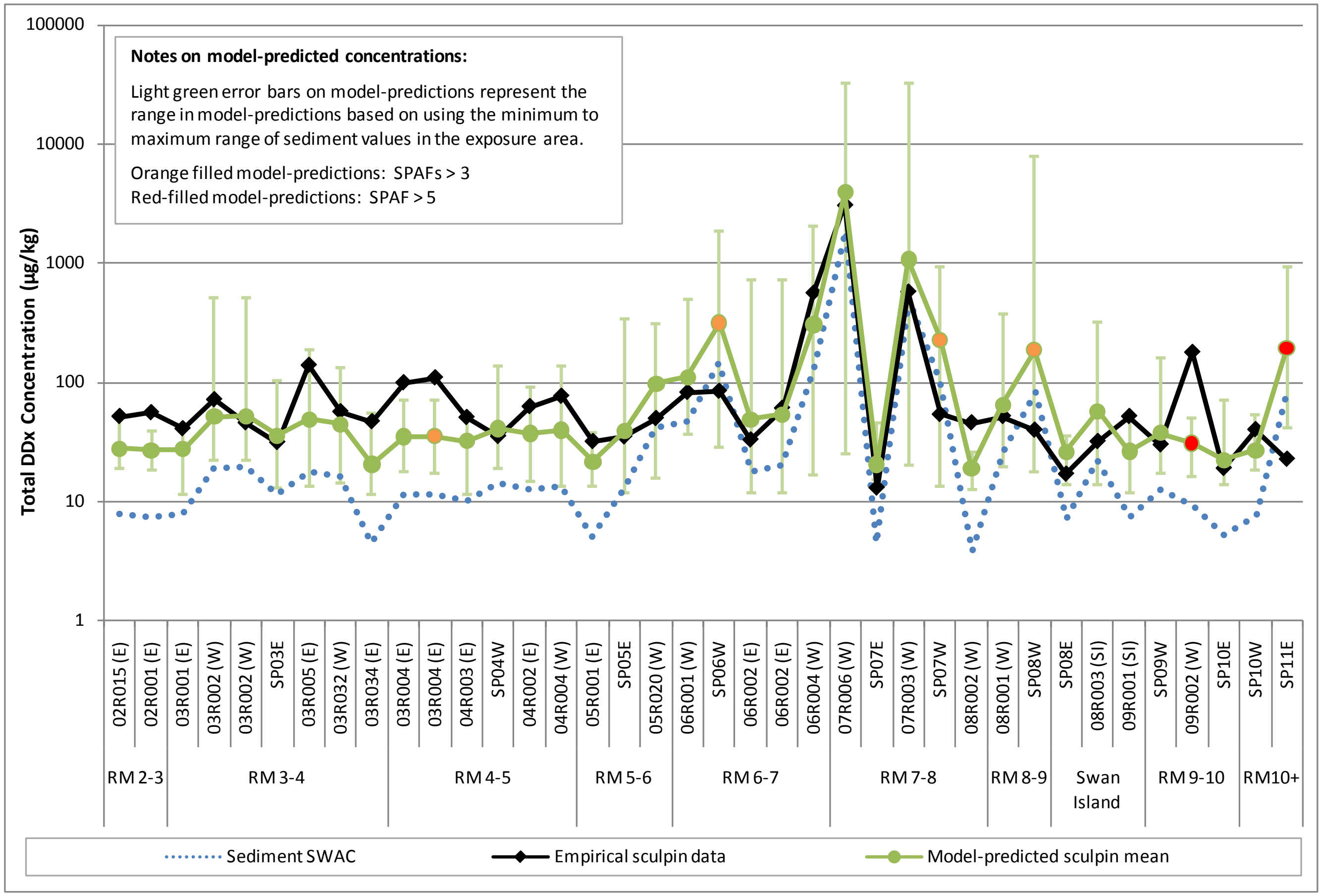


Figure 5-3~~0~~3. Empirical and Model-Predicted Sculpin Tissue Concentrations for Total DDx for RM 2 through RM 11

As with the model predictions for smallmouth bass, the model generally predicted within a factor of 3 compared to the empirical sculpin data based on the mean 0.1-mile-radius SWAC (Figures 5-24~~6~~ to 5-30~~3~~). Again, the error bars based on the range of sediment concentrations in the exposure areas were often larger at sculpin composite locations where the model did not predict as well, and thus the error bars overlapped the empirical sculpin data. This again demonstrates that the model works well when applied at smaller spatial scales for species with home ranges smaller than the site.

5.4.4 PRG Development

PRGs for the BHHRA and BERA were generated using the calibrated model for PCBs, dioxins, and pesticides. PRGs are defined as the sediment SWACs at which the applicable model-predicted tissue concentrations are equal to the target tissue levels. For dietary lines of evidence, a range of PRGs was generated to reflect exclusive consumption of the most- and least-bioaccumulating species that could be modeled. PRGs were calculated by assuming background water concentrations (Table 5-15). The background water concentration values are reflective of upstream concentrations as used in the Early PRG report (Windward et al. 2009).

Table 5-15. Chemical Concentration in Study Area and Background Water

	Dissolved Water Concentration (ng/L)	
Chemical	**Calibrated Study Area-Wide Value**	**Background Value[a]**
PCBs		
Total PCBs[a]	0.228	0.105
PCB 77	0.000260	0.000128
PCB 126	1.25×10^{-5}	1.51×10^{-5}
~~**Dioxins and Furans**~~		
~~2,3,4,7,8-PeCDF~~	~~6.37×10^{-6}~~	~~2.04×10^{-6}~~
Pesticides		
4,4′-DDD	0.053	0.021
4,4′-DDE	0.031	0.030
4,4′-DDT	0.015	0.026
Aldrin	0.0023	0.0016
alpha-HCH	0.017	0.019
beta-HCH	0.0053	0.0034
Dieldrin	0.076	0.080
gamma-HCH	0.028	0.022
Heptachlor	0.00019	0.00073
Heptachlor epoxide	0.0072	0.0091

Table 5-15. Chemical Concentration in Study Area and Background Water

	Dissolved Water Concentration (ng/L)	
Chemical	Calibrated Study Area-Wide Value	Background Value[a]
Sum DDD	0.094	0.027
Sum DDE	0.038	0.031
Sum DDT	0.0217	0.032
Total chlordane	0.031	0.030
Total DDx	0.139	0.0897

[a] Dissolved background water concentrations for use in the mechanistic model were calculated using the same method as was used for total background water concentrations presented in the Portland Harbor RI/FS draft final remedial investigation report (Integral et al. 2011).

DDD – dichlorodiphenyldichloroethane
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
HCH – hexachlorocyclohexane
PCB – polychlorinated biphenyl
~~PeCDF – pentachlorodibenzofuran~~
total DDx – sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE and 4,4′-DDT)

Early PRGs calculated using the mechanistic model were provided in the Early PRG Report (Windward et al. 2009). PRGs were calculated based on the BHHRA for both child and adult Tribal and non-Tribal consumption scenarios. Diets evaluated in the BHHRA included single-species diets of clams, crayfish, smallmouth bass, black crappie, brown bullhead, and carp and a multispecies diet consisting of 25% of each fish species. Details regarding these scenarios can be found in the BHHRA. For the BERA, PRGs were calculated based on tissue residue TRVs for fish and benthic invertebrates (clams, crayfish, and worms) and on dietary TRVs for fish, birds, and mammals. Details regarding these ecological receptors and the diets (when applicable) can be found in the BERA.

5.5 SENSITIVITY ANALYSIS

A complete model sensitivity analysis was done for the model developed as part of the Round 2 Report using Crystal Ball® software's sensitivity analysis function. Because the model structure was not significantly altered from Round 2 Report model, a full sensitivity analysis was not performed. Section 5.5.1 summarizes the Round 2 Report model sensitivity analysis findings, and Section 5.5.2 looks at the relative contributions of water and sediment to model-predicted tissue concentrations.

5.5.1 Summary of Round 2 Report Sensitivity Analysis

As part of the Comprehensive Round 2 Report (Integral et al. 2007), a sensitivity analysis was performed for the model using the Crystal Ball® software's sensitivity analysis function, which includes consideration of the uncertainty of a parameter's input values and the effect that a change in that parameter value has on model-predicted tissue concentrations (based on the model's mathematical formulas). In this type of analysis, sensitivity is calculated by Crystal Ball® as a rank correlation coefficient between each input parameter and the predicted tissue concentration, which is then standardized so that all parameters will together equal 100% of the possible variance. This analysis allows for the identification of the most sensitive model parameters (i.e., those with the largest impact on model predictions). Because no major changes in model structure occurred between the Round 2 Report and the updated model, a full sensitivity analysis was not repeated for the updated model. Instead, a summary of the Round 2 Report analysis is provided here. Full results of this analysis were presented in Appendix ~~D~~ B and Attachment E6 of the Comprehensive Round 2 Report (Integral et al. 2007).

Based on the Round 2 Report sensitivity analysis, it was possible to determine which parameters were most important to model predictions. This summary focused on parameters that consistently contributed 5% or more to variance in model predictions for several modeled species. The most consistently important parameter (across species and chemicals, with and without sediment variability) was the K_{OW}. Generally, the K_{OW} was more important with increasing trophic level and with increasing K_{OW}. When sediment chemical concentration was allowed to vary, the importance of the K_{OW} to model predictions was generally reduced. Sediment chemical concentration, when allowed to vary, was very important for all trophic groups other than plankton (plankton only bioaccumulated chemicals via water in the mechanistic model). Chemical concentration in filtered water was consistently important for plankton. Water temperature was shown to be consistently important, particularly for fish groups.

The lipid fraction for benthic invertebrate consumers, which ranged widely (from 0.008 to 0.42), was important both for benthic invertebrate consumers and for many fish groups that consume them. This wide range was much broader than the lipid fraction range for most other trophic groups, due largely to the fact that benthic invertebrate consumers were intended to reflect a large and diverse group of organisms (benthic worms, insect larvae, and amphipods).

Several additional parameters were less consistently important across species and chemicals. Despite defining the dietary consumption parameters with broad ranges of values, (often spanning 50% or more of total diet; see Appendix ~~D~~B), dietary assumptions were only important for certain species-chemical combinations. Only for northern pikeminnow and largescale sucker did dietary consumption parameters contribute more than 10% to the total predicted chemical concentration differences for some chemicals. Dietary consumption parameters for most other species and chemicals contributed well below 5%. Lipid fraction and water content fraction were sometimes important for their associated modeled group (i.e., common carp lipid content to common carp predicted tissue concentration) for some chemicals. Porewater ventilation was sometimes important for benthic invertebrate filter feeders and sculpin, which consume large amounts of benthic invertebrates.

Several parameters, including the dietary absorption efficiency of lipids for EICs and the NLOM-proportionality constant, were found to be somewhat important in the Round 2 Report sensitivity analysis. However, based on EPA comments on the Comprehensive Round 2 Report (EPA 2008a), these parameters were not calibrated for this version of the mechanistic model (see Appendix ~~D~~B for additional information). Because of their low importance, not calibrating these parameter values did not significantly affect model performance.

5.5.2 Water and Sediment Contribution

As requested by EPA (2008a), the relative contribution of chemicals in water and sediment to total chemical burden in tissue was evaluated for the calibrated mechanistic model to determine the relative importance of these source media. The contribution from water can occur via direct exposure and via dietary uptake (the portion of dietary uptake that originated as water contamination lower in the food chain). The contribution from sediment can occur via direct sediment consumption, porewater ventilation (the chemical concentration in porewater is calculated from the sediment concentration), and dietary uptake (the portion of dietary uptake that originated as sediment or porewater contamination lower in the food chain). Together, the sediment and water contributions to the model-predicted tissue concentrations account for 100% of estimated chemical concentration in tissue.

Table 5-16 shows the water contribution for each chemical-species combination under current conditions. Because the total concentration of a given chemical in the water column within the Study Area originates from many different inputs (e.g., upstream sources, sediment, stormwater, seeps) the percent water contribution shown in Table 5-16 does not indicate the source of the chemical, just the pathway. Phytoplankton and zooplankton are not shown in this table because the predicted chemical concentrations for these species are based only on the contribution from the water pathway (dissolved, not particulate, 100% contribution for all chemicals for these species). Note that the percent contribution of sediment to tissue concentration is equal to 100 minus the value listed in Table 5-16. For example, under current conditions, 90% of predicted total PCBs in smallmouth bass is attributable to sediment exposure (direct or indirect).

Table 5-16. Water Contribution to Model-Predicted Tissue Concentrations

	Model Input Values			Percent Contribution from Water Pathway[a]							
Chemical	Sediment (µg/kg dw)	Water (ng/L)	K_{OW}	Benthic Invertebrate Filter Feeder	Benthic Invertebrate Consumer	Epibenthic Invertebrate Consumer	Sculpin	Large-scale Sucker	Carp	Small-mouth Bass	Northern Pike-minnow
PCBs											
Total PCBs	92.6	0.228	6.14	13%	7%	12%	10%	11%	11%	10%	11%
PCB 77	0.185	2.6×10^{-4}	6.02	7%	4%	7%	6%	6%	6%	6%	6%
PCB 126	0.0175	1.3×10^{-5}	6.38	5%	2%	4%	4%	4%	4%	4%	4%
~~**Dioxins and Furans**~~											
~~2,3,4,7,8-PeCDF~~	~~0.0115~~	~~6.4×10^{-6}~~	~~6.58~~	~~4%~~	~~2%~~	~~5%~~	~~3%~~	~~5%~~	~~4%~~	~~3%~~	~~4%~~
Pesticides											
4,4′-DDD	6.26	0.053	5.83	26%	16%	27%	23%	24%	25%	24%	25%
4,4′-DDE	3.43	0.031	6.42	40%	24%	37%	32%	36%	34%	33%	33%
4,4′-DDT	14.8	0.015	6.31	7%	3%	6%	5%	5%	5%	5%	5%
Aldrin	0.466	0.0023	4.11	0.7%	0.5%	1.3%	0.8%	6%	7%	6%	8%
alpha-HCH	0.267	0.017	4.08	8%	6%	13%	9%	47%	48%	47%	53%
beta-HCH	1.278	0.0053	3.43	0.1%	0.09%	0.2%	0.1%	5%	5%	5%	6%
Dieldrin	0.536	0.076	5.26	70%	60%	77%	71%	76%	78%	77%	79%
gamma-HCH	0.706	0.028	3.69	2%	2%	4%	2%	34%	35%	35%	41%
Heptachlor	0.216	0.00019	4.04	0.1%	0.08%	0.2%	0.1%	1.2%	1.2%	1.2%	1.5%
Heptachlor epoxide	0.290	0.0072	4.74	12%	9%	19%	14%	28%	30%	30%	34%
Sum DDD	8.89	0.094	5.73	27%	17%	30%	25%	27%	28%	27%	28%
Sum DDE	4.22	0.038	6.45	41%	24%	37%	33%	37%	34%	33%	33%
Sum DDT	17.3	0.0217	6.00	6%	3%	6%	5%	5%	5%	5%	5%
Total chlordane	2.40	0.031	5.63	28%	19%	32%	27%	28%	31%	29%	31%
Total DDx	30.3	0.139	5.91	17%	10%	18%	15%	16%	16%	15%	16%

[a] Water and sediment contribution together account for 100% of the model-predicted chemical concentration in tissue.

DDD – dichlorodiphenyldichloroethane
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
dw – dry weight
HCH – hexachlorocyclohexane
K_{OW} – octanol-water partition coefficient
PCB – polychlorinated biphenyl
~~PeCDF – pentachlorodibenzofuran~~
total DDx – sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE and 4,4′-DDT)

As can be seen in Table 5-16, the percent contribution of water to the model-predicted tissue concentrations varies greatly by chemical and species. Several factors influence the percent contribution from water:

- Chemical concentration in filtered water relative to the chemical concentration in sediment
- Chemical-specific K_{OW}
- Species-specific fraction of porewater ventilated (contribution from porewater is part of the percent contribution from sediment)

When the chemical concentration in sediment is relatively low compared to the concentration in filtered water, as is the case for some of the pesticides (e.g., dieldrin, alpha-HCH, and heptachlor epoxide), water contribution is more important for all modeled species. Assuming a similar relationship between the chemical concentration in sediment and filtered water, the importance of water contribution increases as the K_{OW} value decreases (see Table 5-16).

Differences in the percent contribution of water across species for a given chemical are related both to the K_{OW} and to the fraction of porewater ventilated. Calibrated porewater ventilation fractions are 0.05 for benthic invertebrate filter feeders (clams), 0.07 for benthic invertebrate consumers (worms), 0.03 for EICs (crayfish), and 0.04 for sculpin. No porewater ventilation was assumed for the other modeled species, although porewater may be important for these species through dietary uptake. Because the chemical concentration in porewater is calculated from the sediment concentration in the model, the contribution from porewater is included in the percent contribution from sediment. Thus, the percent contribution from water will be lower when the percent contribution from porewater is higher.

For any given sediment and water concentrations, the percent contribution of porewater (sediment) to the model-predicted tissue concentration increases as the K_{OW} decreases, thus lowering the percent contribution from water. It should be noted that overall bioaccumulation of chemicals also decreases as the K_{OW} decreases. As can be seen in Table 5-16, at mid-range K_{OW}s (approximately 5 to 7), the contribution from water is similar across species, indicating that the percent contribution from porewater is relatively low. However, at lower K_{OW}s (less than 4.5), the contribution from sediment increases (and therefore the water contribution decreases as shown in Table 5-16) for invertebrates and sculpin (the species that directly ventilate porewater) because of the increased importance of the contribution from porewater ventilation.

While not as important as the three factors highlighted above, the dietary assumptions for each species also determine the percent contribution of water and sediment. EICs (crayfish) have the lowest fraction of porewater ventilated of the four species that directly ventilate porewater, and the highest consumption of plankton (which accumulate chemicals only from water). For these reasons, EICs generally have the highest percent contribution from water of the four species that directly ventilate porewater. Similarly, northern pikeminnow, which consume the highest percentage of crayfish of any of the modeled fish species (30%), have a slightly higher percent contribution from water.

5.6 UNCERTAINTY ASSESSMENT

This section discusses the uncertainties inherent in the modeling process, and uses several approaches to evaluate model uncertainty.

5.6.1 Uncertainties Inherent in Modeling

A commonly expressed disadvantage of modeling is the need to define values that may be highly uncertain for the required input parameters. The Arnot and Gobas (2004) mechanistic model is no exception. Distributions must be defined for numerous environmental, chemical, and species-specific parameters before the model can be used. Even when site-specific data are available for a given parameter (as is the case for many of the Arnot and Gobas parameters for the Lower Willamette River model), uncertainty regarding the calibrated value still exists. This uncertainty can be overcome only by testing the model against numerous datasets collected under various conditions to confirm that the model accurately represents the modeled system.

Additionally, it should be noted that while the calibrated values for parameters that affect bioaccumulation may be uncertain, the mechanistic model still provides important information about how chemicals are bioaccumulated in aquatic ecosystems. While a simple statistical model might be preferred if the intent of modeling was to predict sediment concentrations within the range of data, the use of a mechanistic model allows for extrapolation beyond the dataset when calculating PRGs and allows for modification of assumptions about the contribution of the water pathway. However, the stand-alone mechanistic model is not an appropriate tool for tracking the fate and transport of chemicals in the Study Area (from upstream sources and upland/stormwater inputs), between media (sediment and water), and out of the Study Area. The stand-alone mechanistic model cannot determine the sources of chemicals in the water column and in the sediment.

Another possible criticism of the mechanistic model is that it is possible for the model to predict a relationship between sediment and tissue concentrations even if no such relationship is apparent in empirical data. While it is possible that the model may be misrepresenting the bioaccumulation process for a given chemical, much evidence exists in scientific literature that bioaccumulation occurs for persistent hydrophobic organic chemicals of the sort that were included in the mechanistic model described in this bioaccumulation modeling report. . Thus, if no bioaccumulation relationship appears to exist for persistent hydrophobic organic chemicals based on the empirical dataset, it is probably caused by uncertainties in the empirical dataset used to examine the relationship. Often in aquatic systems, quantifying the chemical concentrations to which an organism might have been exposed (e.g., chemical concentration in sediment) is highly uncertain.

This is especially true for medium-home-range species such as smallmouth bass or sculpin because the location where these species were caught does not represent their home range, nor does the Study Area-wide sediment concentration (see Section 3.3.3). Thus, incorrect assumptions about sediment exposure concentrations might result in an incorrect bioaccumulation model. The risk of this happening is greatest for a BSAR, which relies most heavily on co-located data. BSAFs are less vulnerable to this source of uncertainty, but BSAFs for small- or medium-home-range species are inappropriate when, as in Portland Harbor, the relationship between tissue and sediment concentrations varies as a function of sediment concentration (Burkhard 2006). Mechanistic modeling reduces this source of uncertainty because the model is calibrated site-wide, tested at smaller spatial scales with spatially explicit accounting for sediment exposure uncertainty, and verified by applying it to multiple chemicals with varying spatial distributions and physical properties that affect bioaccumulation potential. Additionally, it should be noted that if there is truly no relationship between sediment and tissue concentrations for a bioaccumulative chemical, only a mechanistic model such as the food web model (Arnot and Gobas 2004) can explain this (e.g., by demonstrating the importance of non-sediment sources or the effect of metabolism on tissue concentrations).

5.6.2 Application of the Model for Other Tissue Data

As discussed in Section 5.3.1, the mechanistic model is based on a simplified Lower Willamette River food web. Rather than modeling all species, trophic groups were modeled, with a single species used to represent each trophic group in the model (e.g., smallmouth bass represent small piscivorous fish).

By using representative species to model an entire trophic group, uncertainties are introduced into model predictions for those species that are not directly modeled. PRGs based on black crappie, brown bullhead, and peamouth were needed for either the BHHRA or BERA, and thus the model was applied for these species using their surrogates (Table 5-17). Peamouth and black crappie were modeled as foraging fish (represented by sculpin) and brown bullhead were modeled as benthivorous fish (represented by largescale sucker).

Table 5-17. Comparison of Empirical and Mechanistic Model-Predicted Tissue Concentrations for Species Not Directly Modeled

	Brown Bullhead				Black Crappie				Peamouth			
		Tissue Concentration (µg/kg ww)				Tissue Concentration (µg/kg ww)				Tissue Concentration (µg/kg ww)		
Parameter Name	**DF**	**Empirical**	**Model-Predicted[a]**	**SPAF**	**DF**	**Empirical**	**Model-Predicted[a]**	**SPAF**	**DF**	**Empirical**	**Model-Predicted[a]**	**SPAF**
PCB 77	6/6	0.0472	0.23	**(4.9)**	4/4	0.299	0.30	**(1.0)**	ND	ND	NA	NA
PCB 126	6/6	0.0271	0.031	**(1.1)**	4/4	0.0175	0.046	**(2.6)**	ND	ND	NA	NA
Total PCBs	6/6	511	610	**(1.2)**	4/4	164	350	**(2.1)**	4/4	190	350	**(1.8)**
~~23478-PeCDF~~	~~6/6~~	~~0.000822~~	~~0.0026~~	~~**(3.2)**~~	~~4/4~~	~~0.000275~~	~~0.0049~~	~~**(18)**~~	~~ND~~	~~ND~~	~~NA~~	~~NA~~
4,4′-DDD	6/6	9.4	28	**(2.9)**	4/4	12	14	**(1.2)**	4/4	23	14	1.6
4,4′-DDE	6/6	47	48	**(1.0)**	4/4	56	28	2.0	4/4	130	28	4.6
4,4′-DDT	5/6	20	13	1.5	3/4	9.2	26	**(2.8)**	2/4	4.9	26	**(5.3)**
Aldrin	0/6	1.8	ISD	ISD	0/4	0.54	ISD	ISD	0/4	0.61	ISD	ISD
alpha-HCH	0/6	1.2	ISD	ISD	1/4	0.73	ISD	ISD	0/4	0.5	ISD	ISD
beta-HCH	0/6	1.9	ISD	ISD	0/4	1.1	ISD	ISD	0/4	1.6	ISD	ISD
Dieldrin	2/6	2.5	ISD	ISD	1/4	2.8	ISD	ISD	0/4	1.1	ISD	ISD
gamma-HCH	3/6	2	ISD	ISD	0/4	0.64	ISD	ISD	0/4	1.1	ISD	ISD
Heptachlor	0/6	1.8	ISD	ISD	1/4	0.86	ISD	ISD	0/4	0.84	ISD	ISD
Heptachlor epoxide	0/6	1.3	ISD	ISD	0/4	0.5	ISD	ISD	0/4	0.5	ISD	ISD
Sum DDD	6/6	13	33	**(2.5)**	4/4	14	17	**(1.2)**	4/4	25	17	1.4
Sum DDE	6/6	49	62	**(1.3)**	4/4	57	37	1.5	4/4	140	37	3.8
Sum DDT	5/6	27	19	1.4	3/4	13	26	2.0	2/4	7.2	26	3.6

Table 5-17. Comparison of Empirical and Mechanistic Model-Predicted Tissue Concentrations for Species Not Directly Modeled

	Brown Bullhead				Black Crappie				Peamouth			
		Tissue Concentration (µg/kg ww)				Tissue Concentration (µg/kg ww)				Tissue Concentration (µg/kg ww)		
Parameter Name	**DF**	**Empirical**	**Model-Predicted[a]**	**SPAF**	**DF**	**Empirical**	**Model-Predicted[a]**	**SPAF**	**DF**	**Empirical**	**Model-Predicted[a]**	**SPAF**
Total chlordane	4/6	19	7.5	2.5	4/4	11	4.0	2.8	2/4	9	4.0	2.3
Total DDx	6/6	88	140	1.6	4/4	84	74	1.1	4/4	170	74	2.3

[a] Model predictions for brown bullhead were for benthivorous fish (as represented by largescale sucker in the mechanistic model). Model predictions for black crappie and peamouth were for foraging fish (as represented by sculpin in the mechanistic model).

[a] **(SPAFs)** shown in **bold** and in parentheses indicate that the model was over-predicting for this species-chemical combination.

DDD – dichlorodiphenyldichloroethane
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
DF – detection frequency
HCH – hexachlorocyclohexane
ISD – insufficient data
NA– not applicable
ND– no data
~~PeCDF – pentachlorodibenzofuran~~
SPAF – species predictive accuracy factor
total DDx – sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE and 4,4′-DDT)
ww – wet weight

The mechanistic model predicts well for brown bullhead, black crappie, and peamouth, modeled using surrogate species (see Table 5-17). The SPAFs for all species-chemical combinations generally were < 3 and were all < 6~~, with one exception~~. ~~The mechanistic model overpredicted by a factor of 18 for 2,3,4,7,8-PeCDF for black crappie (modeled as sculpin). The fact that the model predicted well for 2,3,4,7,8-PeCDF for sculpin (the model overpredicted by a factor of only 2.3), indicates that metabolism or uptake of dioxins by black crappie might be different than that for sculpin, causing inaccurate model predictions (overestimated tissue concentrations) for black crappie.~~

5.6.3 Study Area-Wide Sediment SWAC

As discussed previously in this report, the Study Area-wide sediment SWAC was used to calibrate the mechanistic model. Although efforts were made to determine the sediment concentration most representative of Study Area-wide conditions, there is uncertainty regarding this value. To evaluate the impact of this uncertainty on model calibration, the mechanistic model was run 3,000 times assuming two different sediment values each, with distributions defined for the 10 parameters with the most impact on model performance for smallmouth bass (Table 5-18). The two sediment values were equal to the total PCB Study Area SWAC of 92.6 µg/kg dw plus or minus 10% (82.4 and 101.9 µg/kg dw). Table 5-18 presents the calibrated values and the mean, range, and standard deviation of the 10 selected parameters for the top 25 model runs for the low- and high-end sediment concentrations. The top 25 model runs were selected by sorting the model output by the SPAF for smallmouth bass while also limiting SPAFs for other modeled species (similar to the primary model calibration process).

Table 5-18. Sediment SWAC Uncertainty Evaluation

Parameter	Calibrated Value[a]	Low-End Sediment (82.4 µg/kg dw) Mean[b]	Range[b]	SD[b]	High-End Sediment (101.9 µg/kg dw) Mean[c]	Range[c]	SD[c]
General Parameters							
Total PCB log K_{OW}	6.14	6.30	6.13 – 7.70	0.42	6.51	6.09 – 7.78	0.69
Mean water temperature (°C)	13.7	13.0	9.9 – 16.4	1.8	12.3	10.0 – 17.2	1.8
Species-Specific Biological Parameters							
BIC lipid content (fraction)	0.014	0.016	0.010 – 0.039	0.006	0.018	0.008 – 0.035	0.007
BIC porewater ventilation (fraction)	0.07	0.04	0.012 – 0.10	0.03	0.05	0.01 – 0.10	0.03
SMB weight (kg)	0.35	0.37	0.17 – 0.70	0.14	0.41	0.16 – 0.88	0.18
Species-Specific Dietary Parameters							
BIC consumption of sediment	91%	92%	88 – 99%	4%	92%	85 – 99%	4%
SCL consumption of BIF	32%	27%	2 – 50%	14%	30%	6 – 49%	12%
SCL consumption of BIC	53%	57%	25 – 87%	16%	59%	29 – 85%	17%
SMB consumption of BIC	24%	19%	2 – 29%	8%	15%	0 – 29%	9%
SMB consumption of EIC	17%	17%	0 – 29%	8%	20%	4 – 30%	6%

[a] Calibrated values for sediment SWAC of 92.6 µg/kg dw.
[b] Mean, range, and SD for top 25 runs for low-end sediment.
[c] Mean, range, and SD for top 25 runs for high-end sediment.

BIC – benthic invertebrate consumer (worms)
dw – dry weight
EIC – epibenthic invertebrate consumer
K_{OW} – octanol-water partition coefficient
PCB – polychlorinated biphenyl
SCL – sculpin
SD – standard deviation
SMB – smallmouth bass

As presented in Table 5-18, the mean values from the top 25 model runs for both the low- and high-end sediment model runs are similar to the calibrated parameter values. The range of values, however, is generally larger, indicating that there is not a unique model calibration that results in good model performance.

5.6.4 Smallmouth Bass and Sculpin Exposure Areas

As presented in Section 5.4.3, the mechanistic model's performance was evaluated for smallmouth bass and sculpin using SWACs assumed to be representative of the exposure for these species (see Section 3.3.3 for details). While attempts were made to ensure that the selected mean SWAC for these species best represented each composite sample, much uncertainty exists regarding the true sediment exposure concentration. First, although the catch location for each individual fish was recorded, that location was not necessarily representative of the home range of that fish. This was especially true for smallmouth bass, which were assumed to have a home range equal to 1 RM; any given fish could have been at the southeast end of its home range, the northwest end, or anywhere in between when captured. This is less of an issue for sculpin, which are believed to have a smaller home range. Second, because each smallmouth bass and sculpin sample was a composite consisting of varying numbers of fish, the SWAC of interest is the average sediment concentration to which that group of fish was exposed.

These SWAC uncertainties are represented in Figures 5-17~~8~~ to 5-23~~5~~ for smallmouth bass, and in Figures 5-24~~6~~ to 5-30~~3~~ for sculpin, by the error bars on the predictions corresponding to each individual composite sample. As discussed in Sections 5.4.3.3 and 5.4.3.4, these error bars were developed based on the range of sediment concentrations in potential exposure areas for the fish in that particular composite sample. Areas in which the sediment concentrations are highly variable have larger error bars, indicating a higher level of uncertainty about the true SWAC to which the composite was exposed. Areas with less variable sediment concentrations have less SWAC uncertainty. Often, composite samples with the greater SWAC uncertainty also had poorer model predictions.

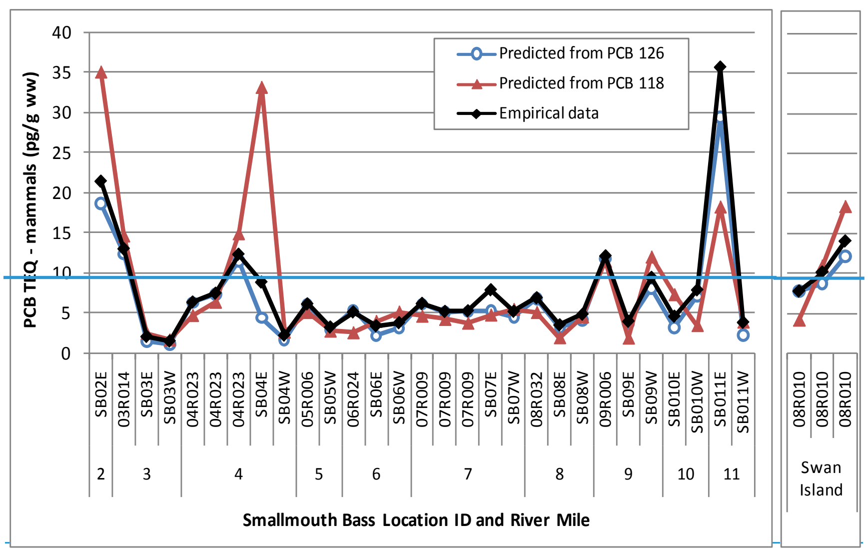
~~5.6.5 Use of Surrogate Chemicals for Modeling TEQs~~

~~As discussed in Section 3.2 and in Appendix A, individual surrogate congeners were selected for PCB and dioxin TEQs. This was necessary because the TEQs represent the toxicity of mixtures comprised of congeners that bioaccumulate differently from one another because of their different physical properties, and thus modeling these TEQ sums~~

~~from abiotic media (sediment and water) to tissue would be inappropriate (EPA 2008c) and highly uncertain.~~

~~While the use of surrogate chemicals is better from a modeling perspective, uncertainty is introduced by the use of surrogate congeners to model the TEQs because of the need to convert between the TEQ units on the target tissue level and the surrogate units for the sediment PRG.~~

~~To evaluate this uncertainty, the PCB TEQ for mammals and the selected surrogate (PCB 126) were selected as an example. Figure 5-34 shows the empirical PCB TEQ mammal data for the smallmouth bass samples compared to the PCB TEQ mammal data predicted from PCB 126 and PCB 118 (another potential PCB TEQ surrogate that was not selected for PRG estimation) using surrogate-TEQ regression relationships.~~



~~**Figure 5-34. Mechanistic Model Uncertainty for PCB TEQ for Mammals in Smallmouth Bass Estimated Using Surrogate Chemicals**~~

~~As can be seen in the figure, the PCB TEQ concentrations predicted from mechanistic modeling of PCB 126 are closer to the empirical data than the PCB TEQ concentrations predicted from mechanistic modeling PCB 118 and use of the regression equations (r^2 of 0.93 and 0.70, respectively). While there is some difference between the PCB TEQ estimates generated from modeling the selected surrogate (PCB 126) and the empirical PCB TEQ data, this uncertainty is minimized because the surrogate congener with the best regression was selected (i.e., PCB 126 was selected over PCB 118). Thus, while the PRG for TEQs are somewhat uncertain because of the need to use a surrogate congener, this~~

~~uncertainty is acceptable because the alternative (modeling the TEQ from abiotic media to tissue) would have been both highly uncertain and inconsistent with EPA's toxicity equivalence methodology framework (EPA 2008c). The use of the surrogate chemicals allowed for the mechanistic model to be used to develop PRGs for the TEQs.~~

5.6.5~~6~~ Inclusion of NJ-Qualified Data for Pesticides

Data that are NJ-qualified indicate that an analyte has been "tentatively identified" and that the detected concentration is approximate. For organochlorine pesticides, NJ-qualified data are often biased high due to interference from PCBs in the sample. In development and calibration of the mechanistic model, all data were used for pesticides, including those that are NJ-qualified. In the sediment datasets for the modeled organochlorines pesticides, NJ-qualified data made up between 2 and 41% of the dataset. To evaluate the effect on the Study Area-wide sediment SWAC if these data were excluded, the SWACs for several example chemicals were recalculated with these data excluded (Table 5-19).

Table 5-19. Study Area-Wide SWACs Calculated With and Without NJ-Qualified Data

Chemical	Count	Detection Frequency	Percent of Data that is NJ-Qualified	Study Area-Wide SWAC (µg/kg dw)	
				All Data	Excluding NJ-Qualified Data
beta-HCH	1083	41%	20%	1.28	0.771
Sum DDE	1125	83%	19%	4.22	3.72
Total chlordane	1083	68%	29%	2.40	2.52
Total DDx	1128	91%	41%	30.3	38.1

DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
dw – dry weight
HCH – hexachlorocyclohexane
NJ – tentatively identified, detected concentration is approximate
SWAC – spatially weighted average concentration
total DDx – sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE and 4,4′-DDT)

While the datasets including the NJ-qualified data have higher non-spatially weighted average concentrations than the corollary datasets without the NJ-qualified data, the changes to the SWAC do not consistently follow this pattern. The removal of the NJ-qualified data causes the SWACs for total chlordane and total DDx to increase while the SWACs for beta-HCH and sum DDE decrease. The changes to these SWACs are predominantly the result of changes to the spatial weighting of individual samples rather than the removal of the NJ-qualified data. In other words, the removal of a random subset of data points from the dataset would likely have a similar effect on the SWAC (i.e., regardless of the relationship between the non-spatially weighted dataset before and after the subset of data are removed, the SWAC could either increase or decrease depending on the location of the removed data points). Based on this analysis, the uncertainty associated with the inclusion of the NJ-qualified data in the datasets used to calculate the sediment SWACs is expected to be low.

5.6.6~~7~~ Uncertainty Associated with the Application of the Mechanistic Model for PRG Development

When discussing sources of uncertainty in the mechanistic model, it is important to consider the model performance implications for calculated PRGs. The subsections below discuss the influence of the selected water concentration and of model calibration on the calculated sediment PRGs.

5.6.6~~7~~.1 Influence of Selected Water Concentration on the PRG

For the PRGs presented in the Early PRG Report (Windward et al. 2009), it was assumed that the chemical concentration in water would be equal to background. The total PCBs PRG for mink was examined to better understand the impact of this assumption on the estimated PRG.

Using the background water concentration for total PCBs (0.105 ng/L) and the dietary percentages presented in the BERA,[18] a total PCB PRG for mink of 31 µg/kg dw was calculated. If the current Study Area-wide water concentration for total PCBs (0.228 ng/L) were used instead, the PCB PRG for mink would instead be 25 µg/kg dw. Thus, when the current water concentration was used (which is approximately double the background concentration), the PRG decreased by nearly 25%. Table 5-20 shows the percent contribution from water to the model-predicted tissue concentrations at current conditions, and using the assumptions for the PRGs described above.

Table 5-20. Percent Contribution of Total PCBs in Water to Predicted Total Tissue Concentrations in Mink Prey Species

			Percent Contribution from Water				
Conditions	Sediment (µg/kg dw)	Water (ng/L)	Crayfish	Sculpin	Largescale sucker	Carp	Smallmouth bass
Current	92.6	0.228	12%	10%	11%	11%	10%
PRG (assuming water is equal to background)	31	0.105	16%	13%	15%	14%	13%
PRG (assuming water is equal to Study Area-wide)	25	0.228	34%	29%	32%	31%	30%

dw – dry weight
PCB – polychlorinated biphenyl
PRG – preliminary remediation goal

[18] For the BERA, it was assumed that mink consume 20% each of crayfish, sculpin, largescale sucker, carp, and smallmouth bass.

Based on current conditions, water contributed an average of 11% of the model-predicted tissue concentration for the species in the mink diet. PCBs in sediment account for the rest of the predicted concentration in tissue. However, as shown in Table 5-20, the relative contribution of water increases when the average sediment concentration is reduced to the PRG. When water concentration was assumed to be equal to background, an average of 14% of the model-predicted tissue concentration in mink prey was from water. When the water was assumed equal to the current Study Area-wide average concentration, an average of 31% of the model-predicted tissue concentration in mink prey was attributable to water.

This analysis was carried through to a hypothetical area of potential concern mapping exercise. Assuming a total PCB sediment PRG of 31 µg/kg dw resulted in 241 acres falling within AOPCs. Assuming a total PCB sediment PRG of 25 µg/kg dw yielded 332 AOPC acres, a 38% increase in AOPC area.

5.6.6~~7~~.2 Influence of Model Calibration on PRG Estimates

In calibration of the mechanistic model, calibrated parameter values were selected based on the SPAFs, which compare model performance to empirical data. While efforts were taken to ensure that selected set of parameters most accurately represented the Lower Willamette River (multiple verification chemicals and spatial scales were used during calibration), it is possible that a different set of parameters could have been selected that, based on the model SPAF, preformed similarly well.

The three most sensitive parameters in the mechanistic model were the K_{OW}, average water temperature, and the lipid content of benthic invertebrate consumers (worms). The model was run probabilistically 5,000 times using Crystal Ball® with distributions defined for these three parameters; all other parameters were held constant at their calibrated values. The criteria used to determine the range of model predictions were model runs that had an SPAF of < 2 for smallmouth bass, an SPAF of < 5 for all other fish species, and a SPAF of < 10 for invertebrates. These SPAF limitations were developed based on the criteria used to calibrate the mechanistic model (i.e., model performance for smallmouth bass was prioritized).

Figure 5-31~~5~~ shows average model-predicted mink prey tissue concentrations (for the weighted mink diet used in the BERA) versus sediment concentration, based on the calibrated mechanistic model (solid red line), and using the range described above (dashed blue lines). To indicate the uncertainty surrounding the sediment PRG, the dietary target tissue level for mink for total PCBs (224 µg/kg ww) is shown on the graph as a solid black line between the range of model PRG predictions.

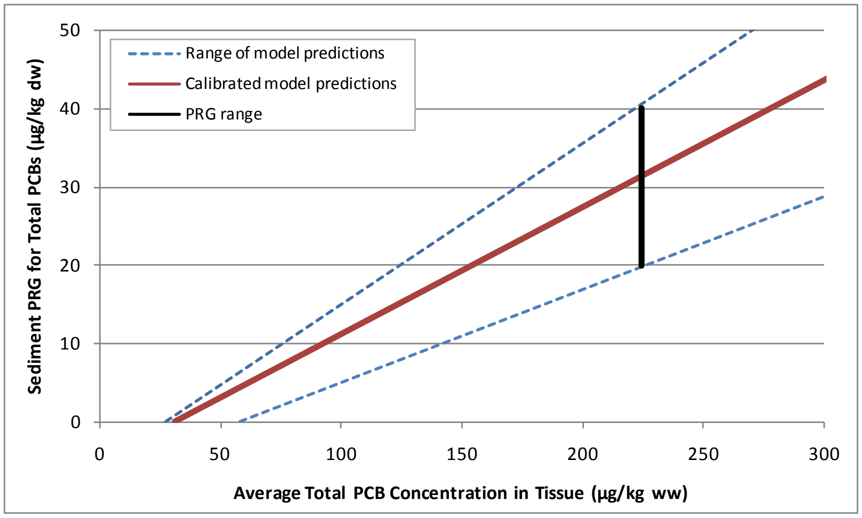


Figure 5-31~~5~~. Mechanistic Model Uncertainty Surrounding the Total PCB PRG for Mink Based on the Average Weighted Diet Used in the BERA

As can be seen in Figure 5-31~~5~~, the PRG for mink of 31 µg/kg dw could potentially range from 20 to 40 µg/kg dw based on calibration uncertainty.

Similarly, Figure 5-32~~6~~ shows the average model-predicted tissue concentrations for smallmouth bass relative to sediment based on the calibrated model, and using the uncertainty range previously described. The figure also shows several target tissue levels for 1 × 10^{-4} excess cancer risk based selected consumption scenarios from the human health risk assessment.

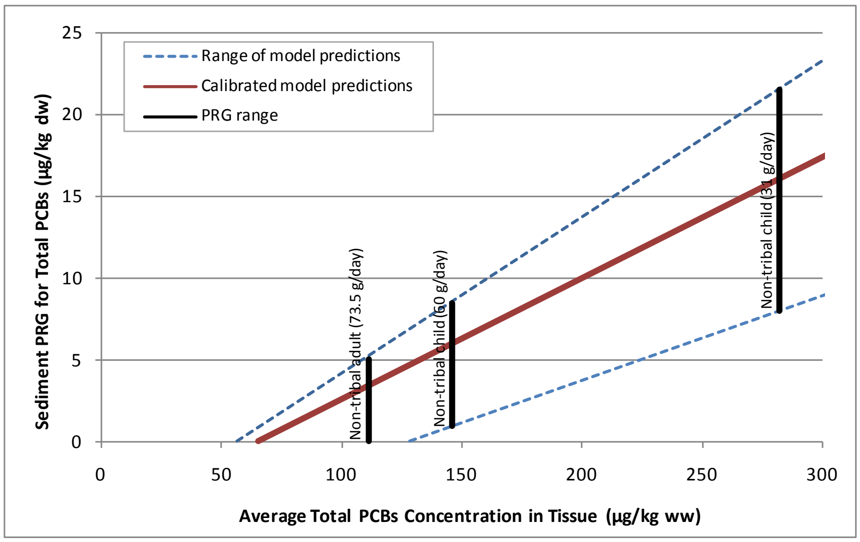


Figure 5-32~~6~~. Mechanistic Model Uncertainty Surrounding Total PCB PRGs for Selected Human Health Scenarios for Excess Cancer Risk of 1 × 10^{-4} Based on the Consumption of Smallmouth Bass

As can be seen in Figure 5-32~~6~~, the uncertainty surrounding the PRGs based on the consumption of smallmouth bass decreases as the target tissue level decreases. The target tissue level for children consuming 31 g/day of smallmouth bass is 282 µg/kg ww for the 1 × 10^{-4} excess cancer risk level, and the corresponding PRG range based on the range of model uncertainty is approximately 8 to 22 µg/kg dw. The lowest target tissue level shown in the figure (111 µg/kg ww for adults consuming 73.5 g/day of smallmouth bass at the 1 × 10^{-4} excess cancer risk level) has a much smaller sediment range, from 0 to 5 µg/kg dw based on the range of model uncertainty.

5.6.6~~7~~.3 Other Factors Influencing the PRG

Another area of uncertainty inherent in the determination of sediment PRGs is the influence of other sources of contamination on fish and invertebrate tissue concentrations. In some cases, the PRG may be biased low because additional sources of contamination (e.g., higher contaminant concentration in the water or the migration of contaminated sediment downstream) may not be fully accounted for. It is more unlikely that sediment PRGs are biased high by these factors, although this may be possible if fish or invertebrate metabolism of a chemical is dependent on the exposure concentration. Some studies have found evidence that fish metabolize certain chemicals at a higher rate when they are exposed to higher chemical concentrations (e.g., dioxins as discussed in Opperhuizen and Sijm (1990)). ~~This theory may help to explain why the model under-predicts for 2,3,4,7,8-PCDF for smallmouth bass at low sediment concentrations but is accurate at~~

~~higher sediment concentrations (Figure 5-21). This would lead to PRGs that were biased low.~~

6.0 MODELING OF ADDITIONAL DIOXIN/FURAN CONGNERS

This section presents the application of the mechanistic model for additional dioxin/furan congeners based on August 14, 2014, and April 10, 2015, requests from EPA. The dioxin/furan congener requested by EPA for inclusion in this report included the following:

- 1,2,3,7,8-Pentachlorodibenzo-*p*-dioxin (pentaCDD)
- 2,3,7,8-Tetrachlorodibenzo-*p*-dioxin (tetraCDD)
- 1,2,3,4,7,8-Hexachlorodibenzofuran (hexaCDF)
- 2,3,4,7,8-Pentachlorodibenzofuran (pentaCDF)
- 2,3,7,8--Tetrachlorodibenzofuran (tetraCDF)

One of these congeners (2,3,4,7,8-pentaCDF) was previously modeled as part of the July 2009 draft of this bioaccumulation modeling report, but has been re-evaluated to ensure that the calibrated values for the chemical-specific parameters are appropriate across the range of dioxin/furan congeners. The subsections that follow present the chemical-specific inputs (Section 6.1), the modeling approach (Section 6.2), and the model results (Section 6.3).

6.1 CHEMICAL-SPECIFIC INPUTS

As was done for the chemicals modeled in Section 5.0, chemical-specific input values were developed for each of the five dioxin/furan congeners modeled in this section. Chemical-specific parameter values for chemical concentration in surface water (Table 6-1), chemical concentration in sediment (Table 6-2), K_{OW} (Table 6-3), and K_M (Table 6-4) were developed for each of the modeled congeners. These parameter values were developed as follows:

- **Chemical concentration in surface water** – The high frequency of non-detects in surface water samples for the dioxin/furan congeners (Table 6-1) created uncertainty regarding true surface water concentrations, so the method used to estimate surface water concentrations was modified for the dioxin/furan congeners (i.e., as compared with the method described in Section 5.3.5.2.1). Two approaches were evaluated (see Appendix B for further details):
  - **Option 1 –** Weighted-average values were calculated as described in Section 5.3.5.2.1, except that half the DL was used for non-detected values (rather than excluding those samples as was done for the other chemicals).
  - **Option 2 –** A second weighted--average water concentration was calculated such that at each step, if no detected values were available, the lowest half DL was used as the average for that step. In addition, the samples collected during the storm event[19] were excluded in order to evaluate the potential

[19] Of the seven events during which water samples were collected, one of these was considered a storm event. See Appendix B for details regarding the water data.

impact of these samples on the estimated overall average water concentration (this was important for sensitivity analysis because the appropriate weight for the storm event was uncertain). This option was used only for those congeners with detection frequencies of less than 50%.

- **Chemical concentration in sediment** – Sediment SWACs were developed using the available sediment chemistry data. The same methods as those described in Section 5.3.5.2.2 were used for the dioxin/furan congeners.
- **K_{OW}** – Chemical-specific K_{OW} values were developed based on the available literature information using the same methods as those described in Section 5.3.5.2.3.
- **K_M** – Metabolic rate constants for fish and invertebrates were derived based primarily on the database of fish biotransformation rates compiled by Arnot et al. (2008).

Additional details regarding the development of these parameter values are provided in Appendix B.

Table 6-1. Chemical Concentrations in Surface Water (NEW)

Analyte	Detection Frequency	Dissolved Water Concentration (ng/L)[a] Option 1 Mean	Option 1 Standard Error	Option 2 Mean	Option 2 Standard Error
Dioxins					
1,2,3,7,8-PentaCDD	8 / 26	4.3×10^{-6}	2.9×10^{-6}	1.5×10^{-6}	5.1×10^{-7}
2,3,7,8-TetraCDD	1 / 26	2.7×10^{-6}	1.2×10^{-6}	8.3×10^{-7}	2.4×10^{-7}
Furans					
1,2,3,4,7,8-HexaCDF	7 / 26	5.9×10^{-6}	1.7×10^{-6}	3.6×10^{-6}	1.2×10^{-6}
2,3,4,7,8-PentaCDF	7 / 26	3.5×10^{-6}	1.2×10^{-6}	2.4×10^{-6}	8.6×10^{-7}
2,3,7,8-TetraCDF	15 / 26	5.5×10^{-6}	1.2×10^{-6}	na	na

Note: Details for the calculation of the weighted average water concentrations are modified from the approach described in Section 5.3.5.2.2 (see bullets above and Appendix B). Non-detected values were assumed to be equal to one-half of the detection limit for dioxins and furans.

[a] The standard error of the data were used to describe the standard deviation of estimates of the mean.

CDD – chlorodibenzo-*p*-dioxin

CDF – chlorodibenzofuran

na – not applicable

Table 6-2. Spatially Weighted Average Concentrations for Chemicals in Sediment (NEW)

Chemical	Detection Frequency	Natural Neighbors SWAC (µg/kg dw)
Dioxins		
1,2,3,7,8-PentaCDD	128 / 219	0.00025
2,3,7,8-TetraCDD	41 / 219	0.00010
Furans		
1,2,3,4,7,8-HexaCDF	197 / 219	0.00271
2,3,4,7,8-PentaCDF	173 / 219	0.0115
2,3,7,8-TetraCDF	145 / 219	0.0168

Note: See Section 5.3.5.2.2 for details regarding the development of this parameter value.
CDD – chlorodibenzo-*p*-dioxin
CDF – chlorodibenzofuran
SWAC – spatially weighted average concentration

Table 6-3. K_{OW} Values for Use in the Model (NEW)

Analyte	log K_{OW} Values	
	Nominal Value	Distribution Range
Dioxins		
1,2,3,7,8-PentaCDD	7.06	6.49 – 7.56
2,3,7,8-TetraCDD	6.38	5.38 – 8.93
Furans		
1,2,3,4,7,8-HexaCDF	7.66	6.92 – 7.92
2,3,4,7,8-PentaCDF	6.95	6.56 – 7.82
2,3,7,8-TetraCDF	6.30	5.82 – 7.70

Note: See Section 5.3.5.2.3 for details regarding the development of this parameter value.
CDD – chlorodibenzo-*p*-dioxin
CDF – chlorodibenzofuran
K_{OW} – octanol-water partition coefficient

Table 6-4. Metabolic Rate Constants (1/day) for Metabolized Chemicals (NEW)

Chemical	Selected K_M Values	
	Nominal Value	Distribution Range
Dixoins		
1,2,3,7,8-PentaCDD	0.019	0.005 – 0.07
2,3,7,8-TetraCDD	0.013	0.002 – 0.08
Furans		
1,2,3,4,7,8-HexaCDF	0.06	0 – 0.6
2,3,4,7,8-PentaCDF	0.058	0.009 – 0.3
2,3,7,8-TetraCDF	0.12	0.01 – 0.5

Source: Arnot et al. (2008); see Appendix B for details.
CDD – chlorodibenzo-*p*-dioxin
CDF – chlorodibenzofuran
K_M – metabolic rate constant

6.2 MODELING APPROACH

This section describes the approach for developing calibrated chemical-specific parameter values for the dioxin/furan congeners. No changes to the calibrated parameter values for the non-chemical-specific parameters were made during this modeling. Because of the importance of considering the relationship between the calibrated values across the various dioxin/furan congeners, a different approach was taken for this calibration (as compared with the approach described in Section 5.3.5.3.2).

Step 1. Consideration of Expectations for Calibrated Parameter Values

The first step in developing calibrated parameter values was to explore the relationship across the congeners with regard to chemical concentrations, K_{OW} values, and K_M values. Table 6-5 summarizes the expectations regarding these relationships and how the calibrated values should compare with one another.

Table 6-5. Calibration Considerations for Dioxins and Furans (NEW)

Parameter	Notes Regarding Calibration
Surface water concentrations	Concentrations of dioxins in water are generally expected to be lower than those of the furans
Sediment concentrations	Concentrations of dioxins in sediment are expected to be lower than those of furans; this is reflected in the parameter values shown in Table 6-2.
K_{OW}	K_{OW} values are expected to increase with increasing chlorination (i.e., the K_{OW} for Hexa > the K_{OW} for Penta > the K_{OW} for Tetra)
K_M	K_M values for dioxins are expected to be lower than those for furans in fish (Loonen et al. 1994).

K_M – metabolic rate constant

K_{OW} – octanol-water partition coefficient

Step 2. Evaluation of Model Performance Using Nominal Values

Nominal parameter values for each of the chemical-specific parameters (i.e., chemical concentration in water, chemical concentration in sediment, K_{OW}, and K_M) were entered in into the model template for each of the five dioxin/furan congeners. For the first attempt at calibration, the Option 1 surface water concentrations were used for all five congeners. Model performance was evaluated relative to the criteria described in Section 5.3.5.3.2 and reproduced here:

- SPAFs for smallmouth bass were < 2, and the percent difference for smallmouth bass was considered to ensure that the model was not under-predicting concentrations for this important species.
- SPAFs for other fish species were considered, and model runs were also sorted to optimize model performance for these species (SPAFs generally < 3).

Table 6-6 presents the uncalibrated model performance. As can be seen in this table, model performance does not meet the specified criteria in most cases.

Table 6-6. Uncalibrated Model Performance for Dioxin and Furan Congeners (NEW)

	SPAF[a]							
Chemical	BIF	EIC	Sculpin	Large-scale Sucker	Carp	Small-mouth Bass	Northern Pikeminnow	Average
Dioxins								
1,2,3,7,8-PentaCDD	- 2.0	+ 1.2	- 1.7	ND	- 9.4	- 7.3	ND	4.3
2,3,7,8-TetraCDD	- 1.9	+ 1.2	+ 1.2	ND	- 4.4	- 1.9	ND	2.1
Furans								
1,2,3,4,7,8-HexaCDF	- 8.0	- 37	- 74	ND	- 73	- 103	ND	59
2,3,4,7,8-PentaCDF	+ 1.9	+ 1.7	+ 2.1	ND	- 1.2	- 2.3	ND	1.9
2,3,7,8-TetraCDF	+ 2.3	+ 1.6	+ 2.6	ND	+ 4.0	+ 4.3	ND	3.0

Note: Uncalibrated model performances use the Option 1 calibrated water concentration for all congeners.

[a] A + or – sign before the SPAF indicates that the model is over-predicting or under-predicting, respectively.

BIF – benthic invertebrate filter feeder
CDD – chlorodibenzo-*p*-dioxin
CDF – chlorodibenzofuran
EIC – epibenthic invertebrate consumer
ND – no data
SPAF – species predictive accuracy factor

Step 3. Selection of Calibrated Parameter Values

Calibrated parameter values were determined by evaluating model performance for the five dioxin/furan congeners in order of decreasing chlorination (i.e., starting with hexa, then penta, and finally tetra congeners). For each congener, the K_{OW} was adjusted to improve model calibration while also maintaining the expected relative relationship of K_{OW} values for the various congeners. Metabolic rates were then adjusted for each congener to improve model performance to meet the standards described above in Step 2.

Once the initial chemical-specific calibration was completed, a second evaluation was conducted for each of the congeners to further optimize model performance for each congener and to ensure that the relationship between the calibrated parameter values across the five congeners were reasonable.

Step 4. Evaluation of Alternate Water Concentrations

Using the calibrated chemical-specific values selected in Step 3, the alternate water concentrations (presented in Table 6-1 as "option 2") were entered into the model for the four dioxin/furan congeners with less than 50% detection frequencies. The chemical-specific parameter values (for K_{OW} and K_M) were adjusted to achieve optimal calibration using the alternate water values.

6.3 MODEL RESULTS

Based on the results of the modeling approach described in Section 6.2, calibrated models for each of the five dioxin/furan congeners were developed. Table 6-7 presents the calibrated parameter values for both Calibration 1 (using the Option 1 water values presented in Table 6-1) and Calibration 2 (using the Option 2 water values presented in Table 6-1). A review of the calibrated parameter values reveals the following:

- K_{OW} values increased with increasing chlorination and were similar for the two penta congeners, as well as for the two tetra congeners.
- Concentrations in sediment and water were generally lower for the dioxins than for the furans.
- K_M values were lower for dioxins than for furans.
- No change in the calibration was necessary for two of the four congeners (1,2,3,4,7,8-hexaCDF and 2,3,4,7,8-pentaCDF) for which alternative water concentrations were evaluated. Thus, the results for these alternative calibrations are not presented. Alternative calibrations are presented only for 1,2,3,7,8-pentaCDD and 2,3,7,8-tetraCDD.

Table 6-8 presents the SPAFs for the calibrated model.

Table 6-7. Summary of Calibrated Chemical-Specific Values for Dioxins and Furans (NEW)

Chemical	Concentration in Dissolved Water (ng/L)	Concentration in Sediment (µg/kg dw)	K_{OW}	K_M for Invertebrates (1/day)	K_M for Fish (1/day)
Calibration 1					
Dioxins					
1,2,3,7,8-PentaCDD	4.3×10^{-6}	0.00025	6.7	0.008	0.008
2,3,7,8-TetraCDD	2.7×10^{-6}	0.00010	6.3	0.007	0.007
Furans					
1,2,3,4,7,8-HexaCDF	5.9×10^{-6}	0.00271	7.0	0.015	0.015
2,3,4,7,8-PentaCDF	3.5×10^{-6}	0.0115	6.6	0.05	0.02
2,3,7,8-TetraCDF	5.5×10^{-6}	0.0168	6.3	0.03	0.03
Calibration 2					
Dioxins					
1,2,3,7,8-PentaCDD	1.5×10^{-6}	0.00025	6.6	0.006	0.006
2,3,7,8-TetraCDD	8.3×10^{-7}	0.00010	6.3	0.005	0.005
Furans					
1,2,3,4,7,8-HexaCDF	3.6×10^{-6}	0.00271	7.0	0.015	0.015
2,3,4,7,8-PentaCDF	2.4×10^{-6}	0.0115	6.6	0.05	0.02

[a] Uniform distributions developed from literature values were used to calibrate the model (see Appendix B for additional information).

[b] Normal distributions based on XAD water samples from the Lower Willamette River were used to calibrate the model (see Appendix B for additional information).

CDD – chlorodibenzo-*p*-dioxin
CDF – chlorodibenzofuran
dw – dry weight
K_M – metabolic rate constant
K_{OW} – octanol-water partition coefficient
SD – standard deviation

Table 6-8. Calibrated Model Performance for Dioxin and Furan Congeners (NEW)

	SPAF[a]							
Chemical	**BIF**	**EIC**	**Sculpin**	**Large-scale Sucker**	**Carp**	**Small-mouth Bass**	**Northern Pikeminnow**	**Average**
Calibration 1								
Dioxins								
1,2,3,7,8-PentaCDD	+ 1.1	+ 2.7	+ 2.0	ND	- 2.5	1.0	ND	1.9
2,3,7,8-TetraCDD	- 1.6	+ 1.4	+ 1.7	ND	- 2.5	+ 1.2	ND	1.7
Furans								
1,2,3,4,7,8-HexaCDF	+ 1.2	- 1.3	- 1.8	ND	- 1.7	1.0	ND	1.4
2,3,4,7,8-PentaCDF	+ 1.8	+ 1.3	+ 3.5	ND	+ 1.5	+ 1.1	ND	1.8
2,3,7,8-TetraCDF	+ 1.4	- 1.2	+ 1.1	ND	+ 1.5	+ 1.1	ND	1.3
Calibration 2								
Dioxins								
1,2,3,7,8-PentaCDD	- 1.3	+ 1.9	+ 1.7	ND	- 2.7	1.0	ND	1.7
2,3,7,8-TetraCDD	- 2.6	- 1.1	+ 1.3	ND	- 3.1	1.0	ND	1.8

[a] A + or – sign before the SPAF indicates that the model is over-predicting or under-predicting, respectively.
BIF – benthic invertebrate filter feeder
CDD – chlorodibenzo-*p*-dioxin
CDF – chlorodibenzofuran
EIC – epibenthic invertebrate consumer
ND – no data
SPAF – species predictive accuracy factor

6.3.1 Model Predictions Compared with Individual Sample Data

As was done in Section 5.4.3.2 for other chemicals, this section presents an evaluation of model performance in which model-predicted tissue concentrations (both Calibration 1 and Calibration 2 for the two dioxin congeners) were graphed along with the empirical tissue dataset (individual sample concentrations, as well as mean and median values for each species). Note that the following abbreviations are used in the graphs for ease of presentation:

- BIF – benthic invertebrate filter feeder (clams)
- BIC – benthic invertebrate consumer (worms)
- EIC – epibenthic invertebrate consumer (crayfish)
- SCL – sculpin
- LSS – largescale sucker
- CAR – carp

- SMB – smallmouth bass
- NPM – northern pikeminnow

Figures 6-1 through 6-5 graphically display the results of calibrated model predictions compared with empirical data for the modeled dioxin and furan congeners. No field-collected empirical data for dioxins and furans were available for benthic invertebrate consumers (worms), largescale sucker, or northern pikeminnow. As can be seen in these figures, the majority of model-predicted tissue concentrations are similar to the average empirical concentrations and are within the range of the empirical data.

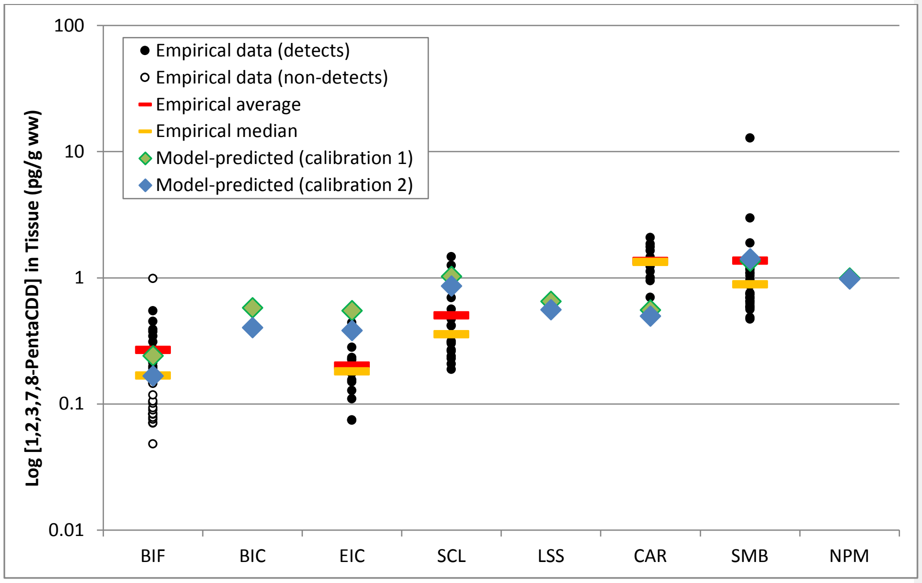


Figure 6-1. Empirical and Model-Predicted Data for 1,2,3,7,8-PentaCDD (NEW)

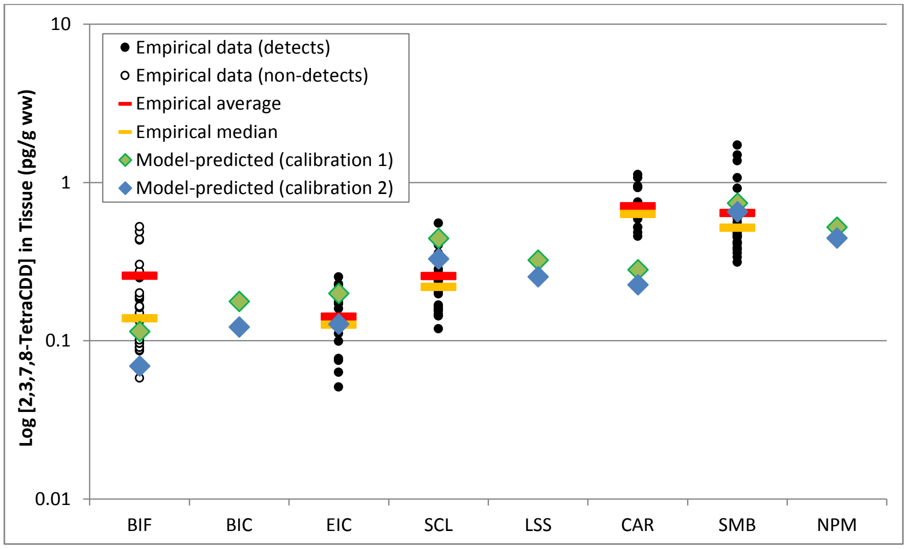


Figure 6-2. Empirical and Model-Predicted Data for 2,3,7,8-TetraCDD (NEW)

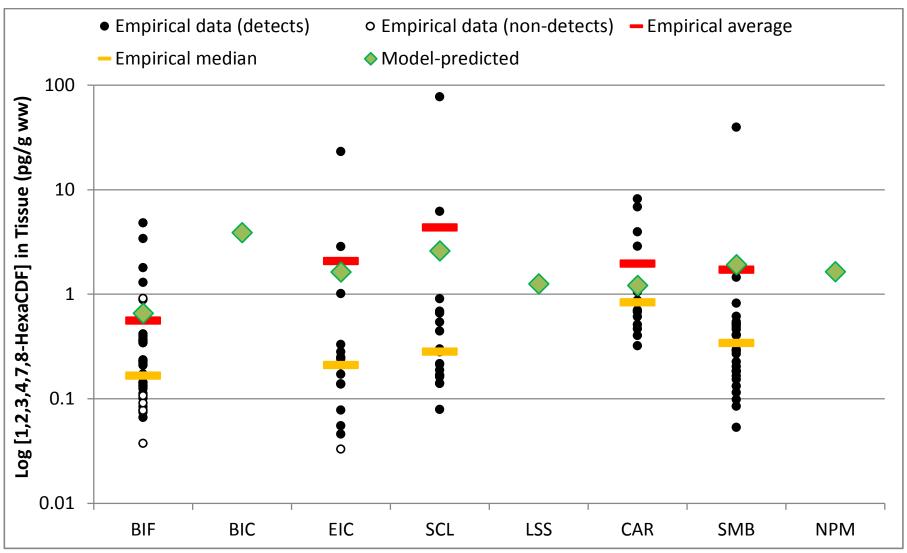


Figure 6-3. Empirical and Model-Predicted Data for 1,2,3,4,7,8-HexaCDF (NEW)

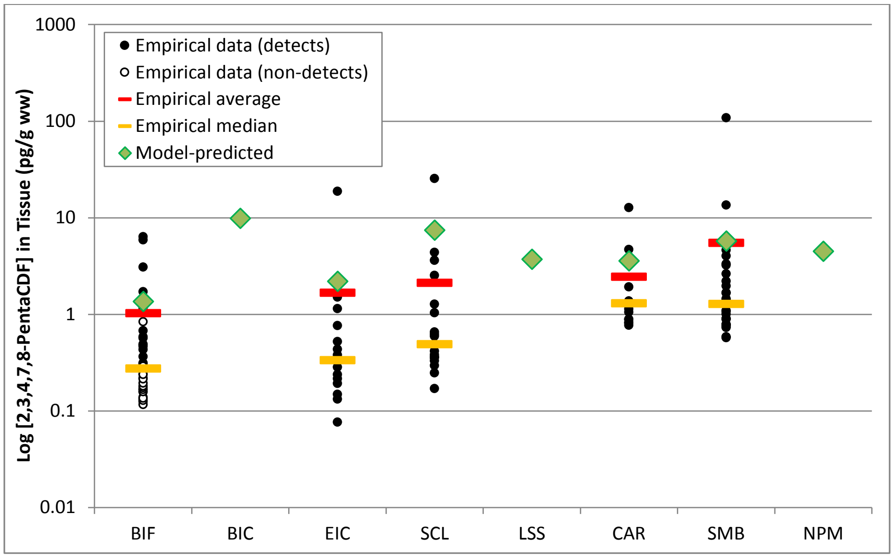


Figure 6-4. Empirical and Model-Predicted Data for 2,3,4,7,8-PentaCDF (NEW)

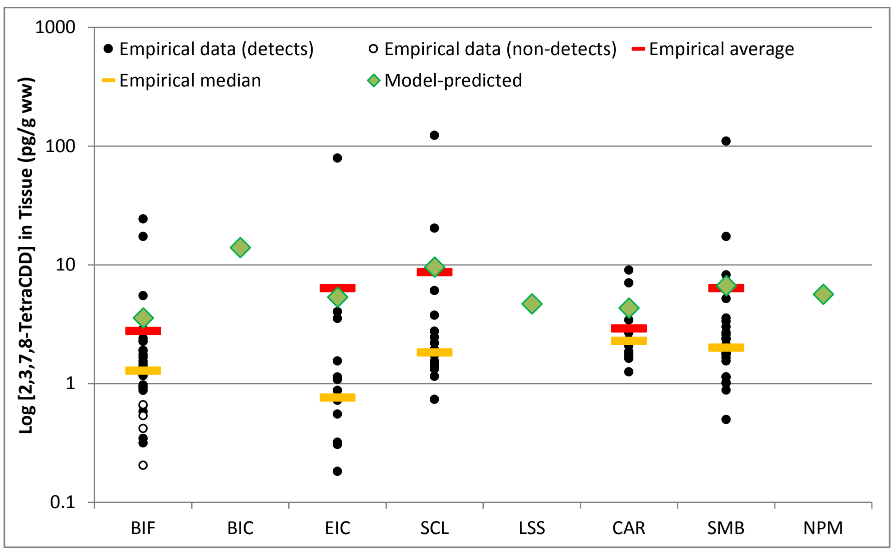


Figure 6-5. Empirical and Model-Predicted Data for 2,3,7,8-TetraCDF (NEW)

6.3.2 Smaller Spatial Scale Model Application for Smallmouth Bass

As was done in Section 5.4.3.3, the calibrated mechanistic model for each dioxin and furan congener was also evaluated at smaller spatial scales for smallmouth bass. Figures 6-6 to 6-10 present model predictions and empirical data for individual bass composites by location for each of the congeners (note that two figures are presented for each of the dioxins to show both the Calibration 1 and Calibration 2 results [labeled as figures a and b, respectively). Predicted and empirical tissue concentrations are on a wet-weight basis, while sediment concentrations are on a dry-weight basis. The vertical gray bar in the figures separates the samples collected from the main stem of the river (RM 2 to RM 11) and the samples collected from for Swan Island Lagoon (these three samples are shown on the right side of the graphs).

As can be seen in Figures 6-6 to 6-10, the mechanistic model generally predicts the empirical data within a factor of 3. Locations where the model does not predict as well based on the mean sediment SWAC are generally those areas with high variability in the sediment, and thus there is a high level of uncertainty in the sediment concentration to which the smallmouth bass in a given composite (and their prey) were exposed. The uncertainty about these model predictions are represented by error bars calculated based on the minimum and maximum 1-RM SWACs that could be applicable to a given smallmouth bass composite (see Section 3.3.3 for more details).

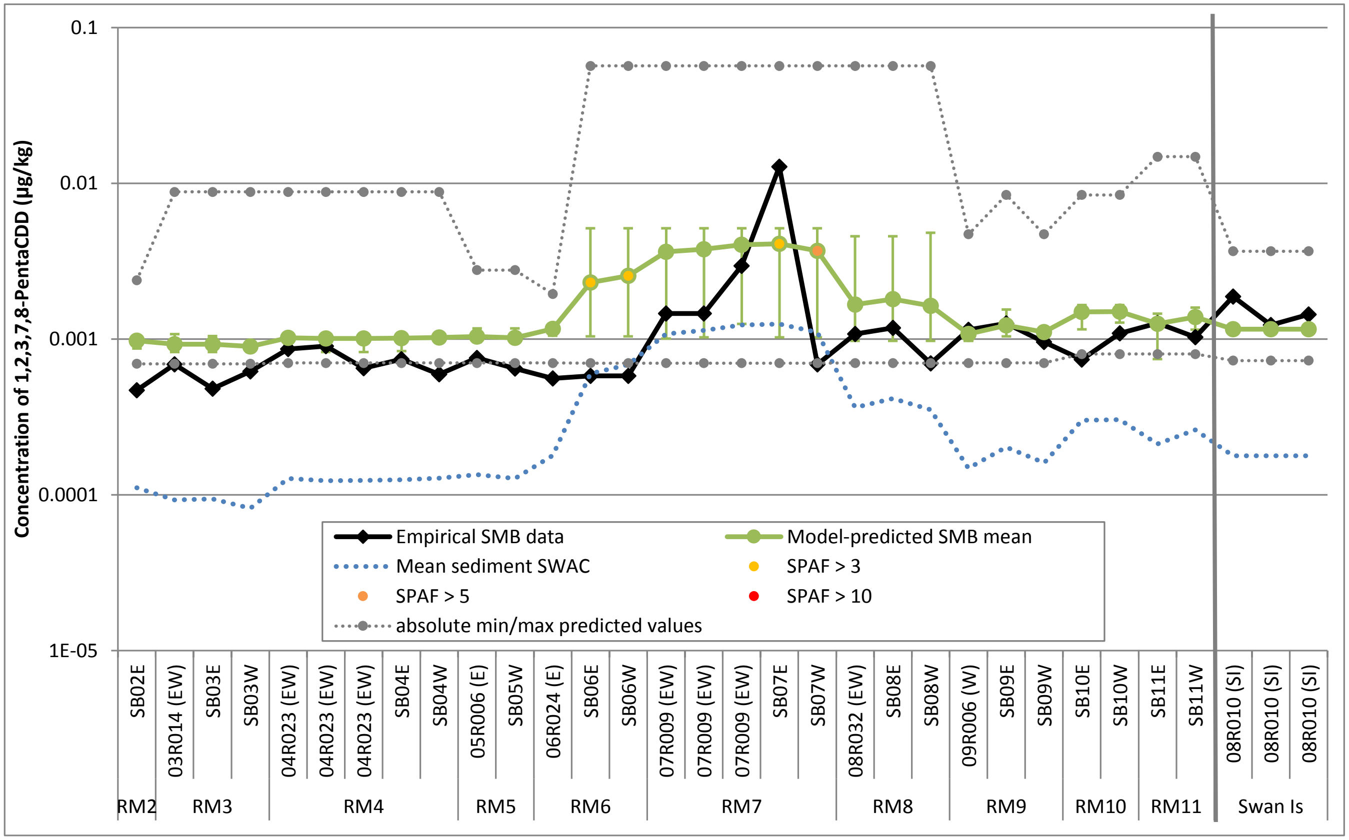


Figure 6-6a. Empirical and Model-Predicted Smallmouth Bass Tissue Concentrations for 1,2,3,7,8-PentaCDD for RM 2 through RM 11 and for Swan Island Lagoon using Calibration 1 (NEW)

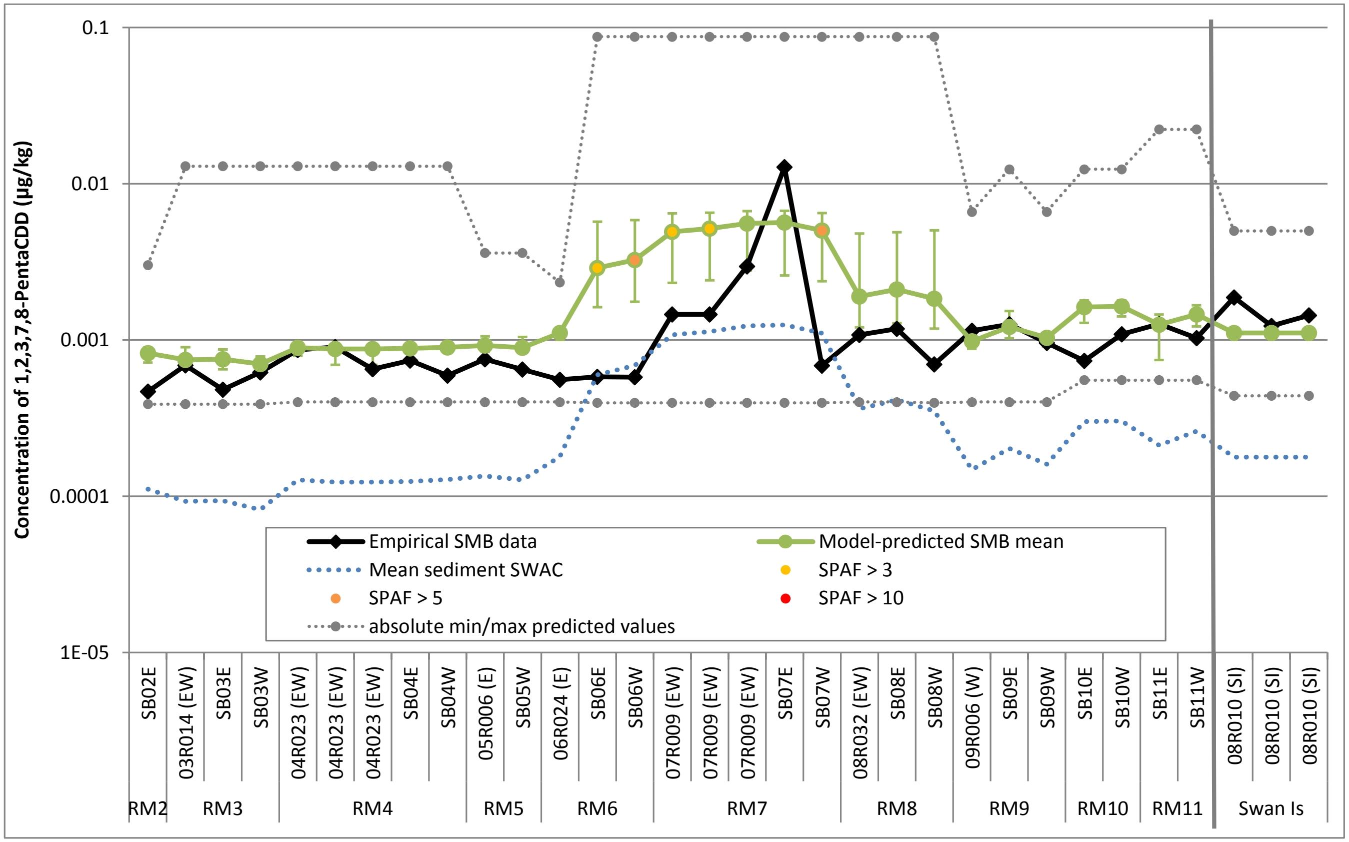


Figure 6-6b. Empirical and Model-Predicted Smallmouth Bass Tissue Concentrations for 1,2,3,7,8-PentaCDD for RM 2 through RM 11 and for Swan Island Lagoon using Calibration 2 (NEW)

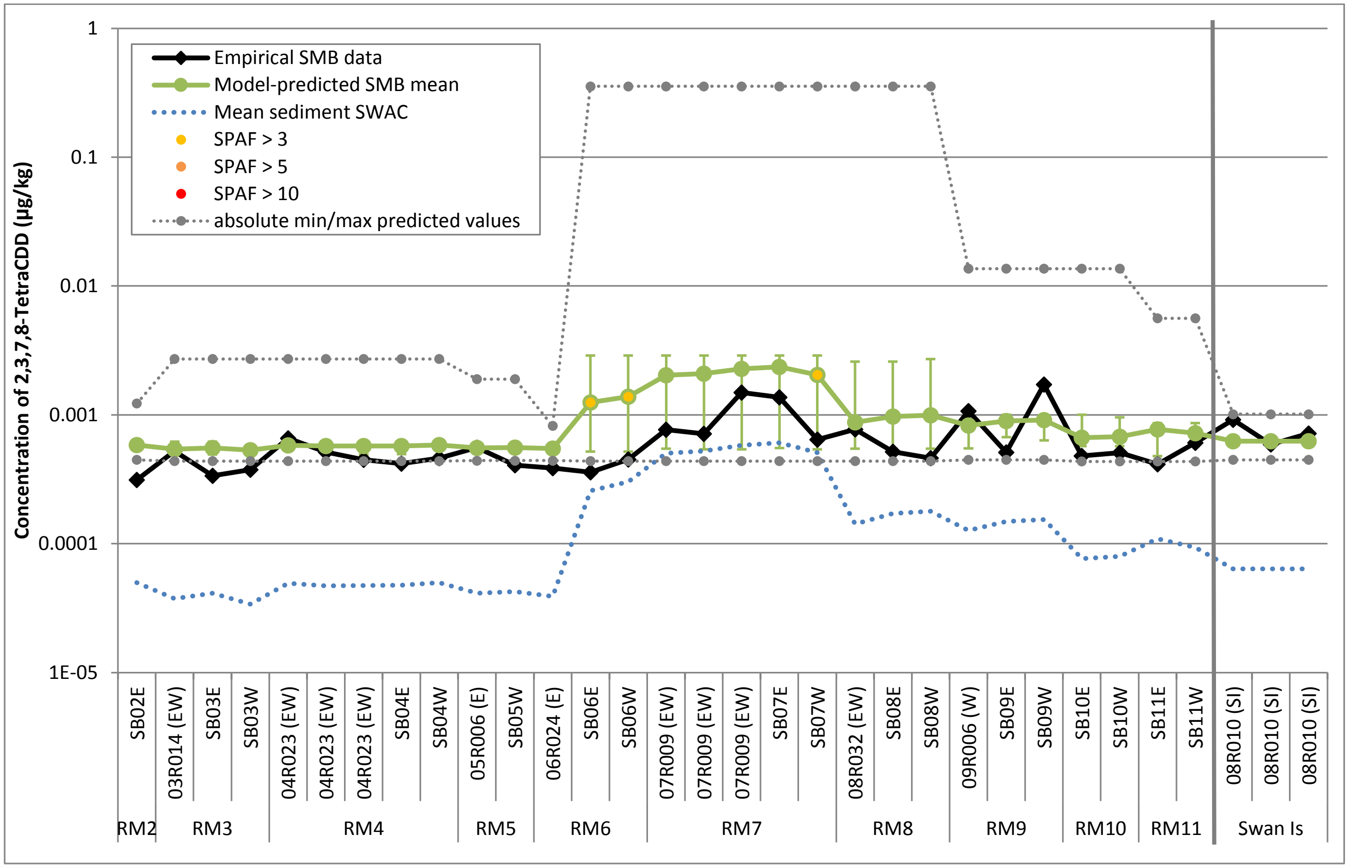


Figure 6-7a. Empirical and Model-Predicted Smallmouth Bass Tissue Concentrations for 2,3,7,8-TetraCDD for RM 2 through RM 11 and for Swan Island Lagoon using Calibration 1 (NEW)

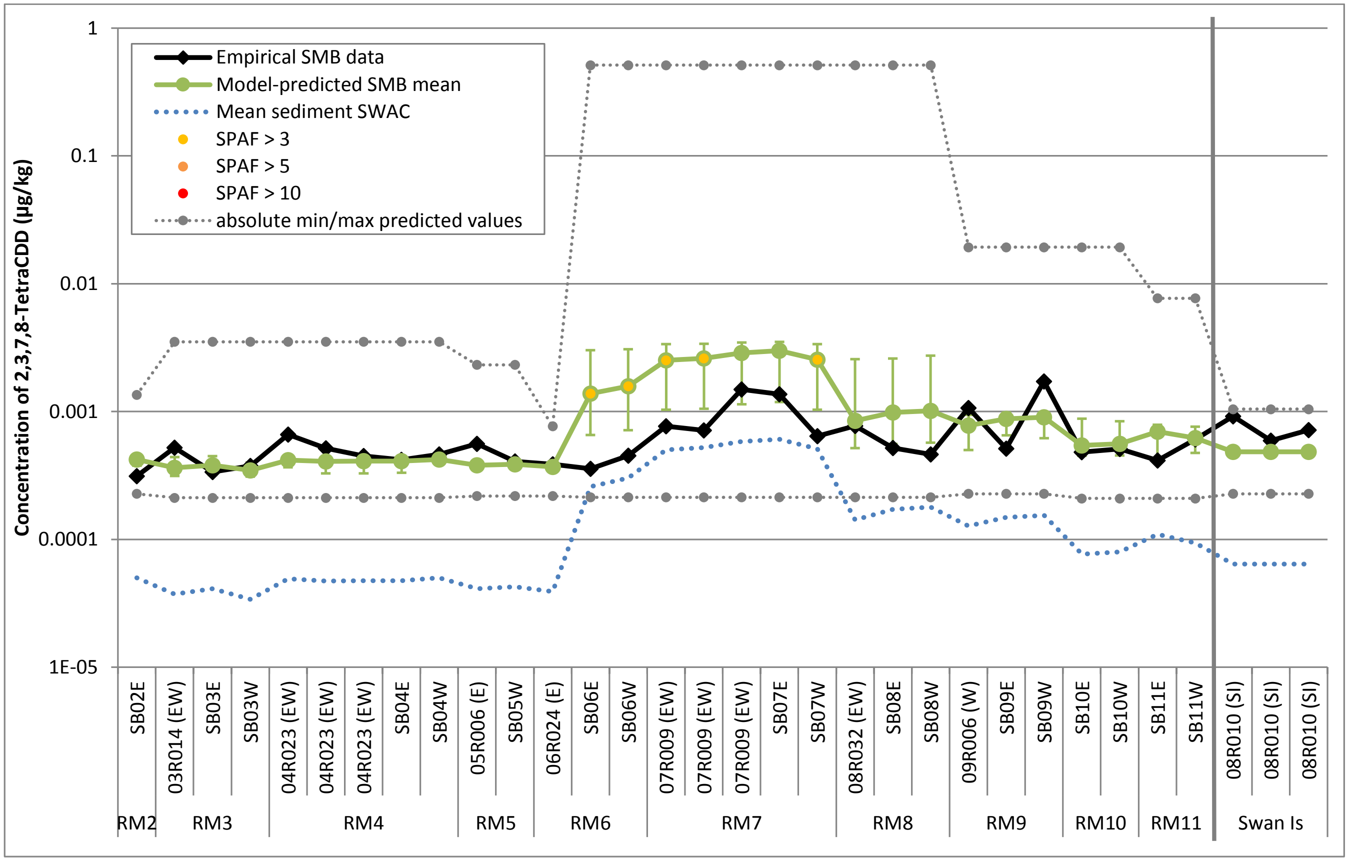


Figure 6-7b. Empirical and Model-Predicted Smallmouth Bass Tissue Concentrations for 2,3,7,8-TetraCDD for RM 2 through RM 11 and for Swan Island Lagoon using Calibration 2 (NEW)

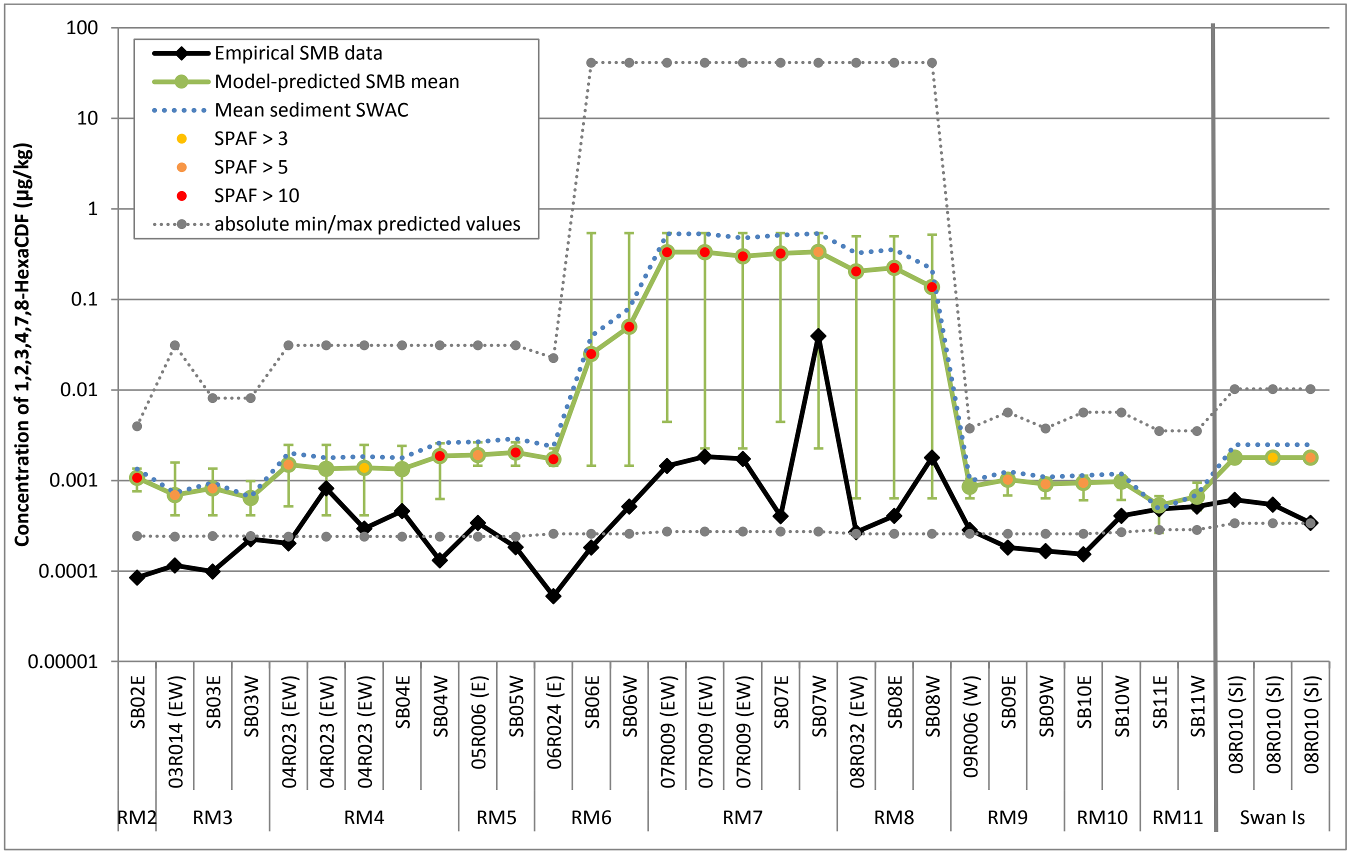


Figure 6-8. Empirical and Model-Predicted Smallmouth Bass Tissue Concentrations for 1,2,3,4,7,8-HexaCDF for RM 2 through RM 11 and for Swan Island Lagoon (NEW)

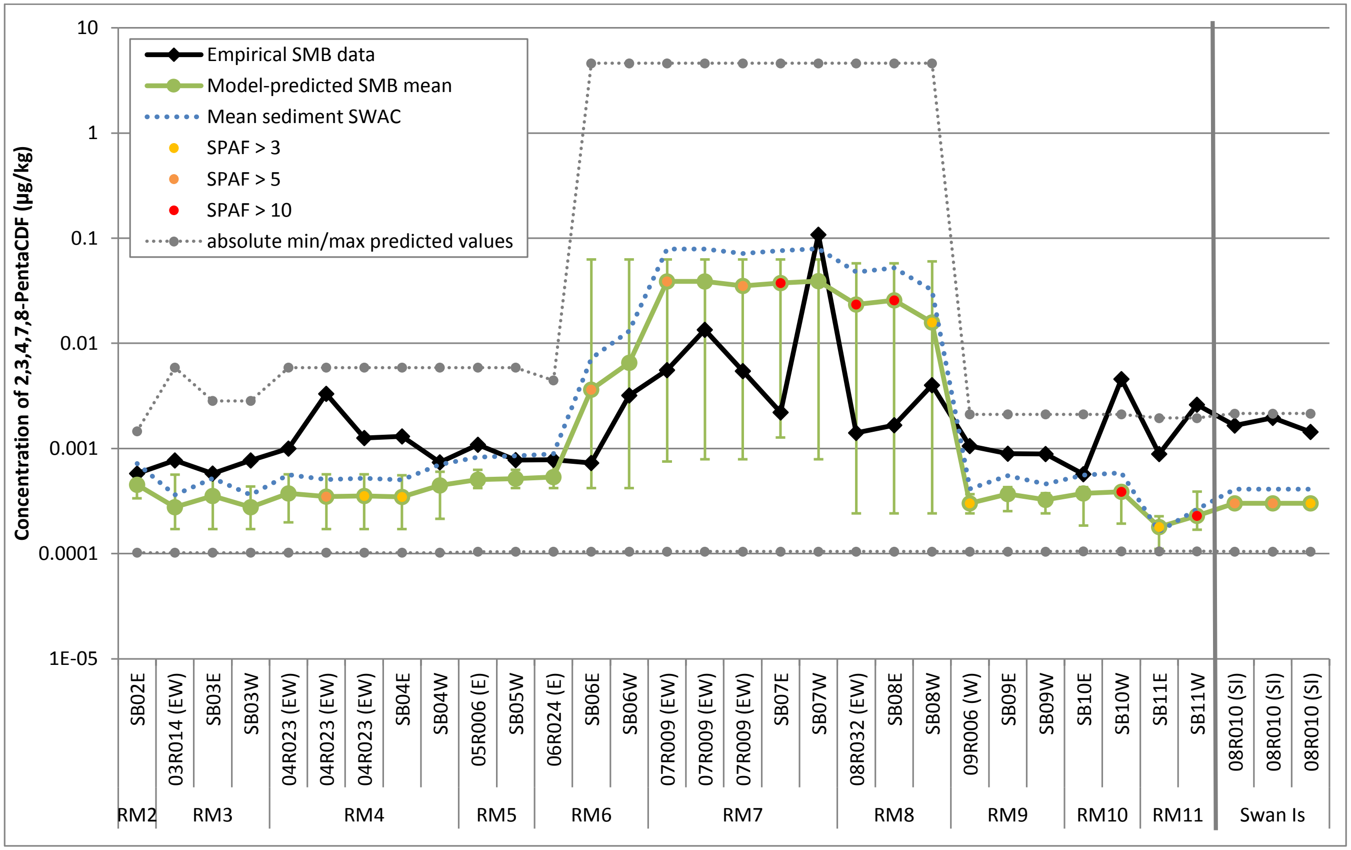


Figure 6-9. Empirical and Model-Predicted Smallmouth Bass Tissue Concentrations for 2,3,4,7,8-PentaCDF for RM 2 through RM 11 and for Swan Island Lagoon (NEW)

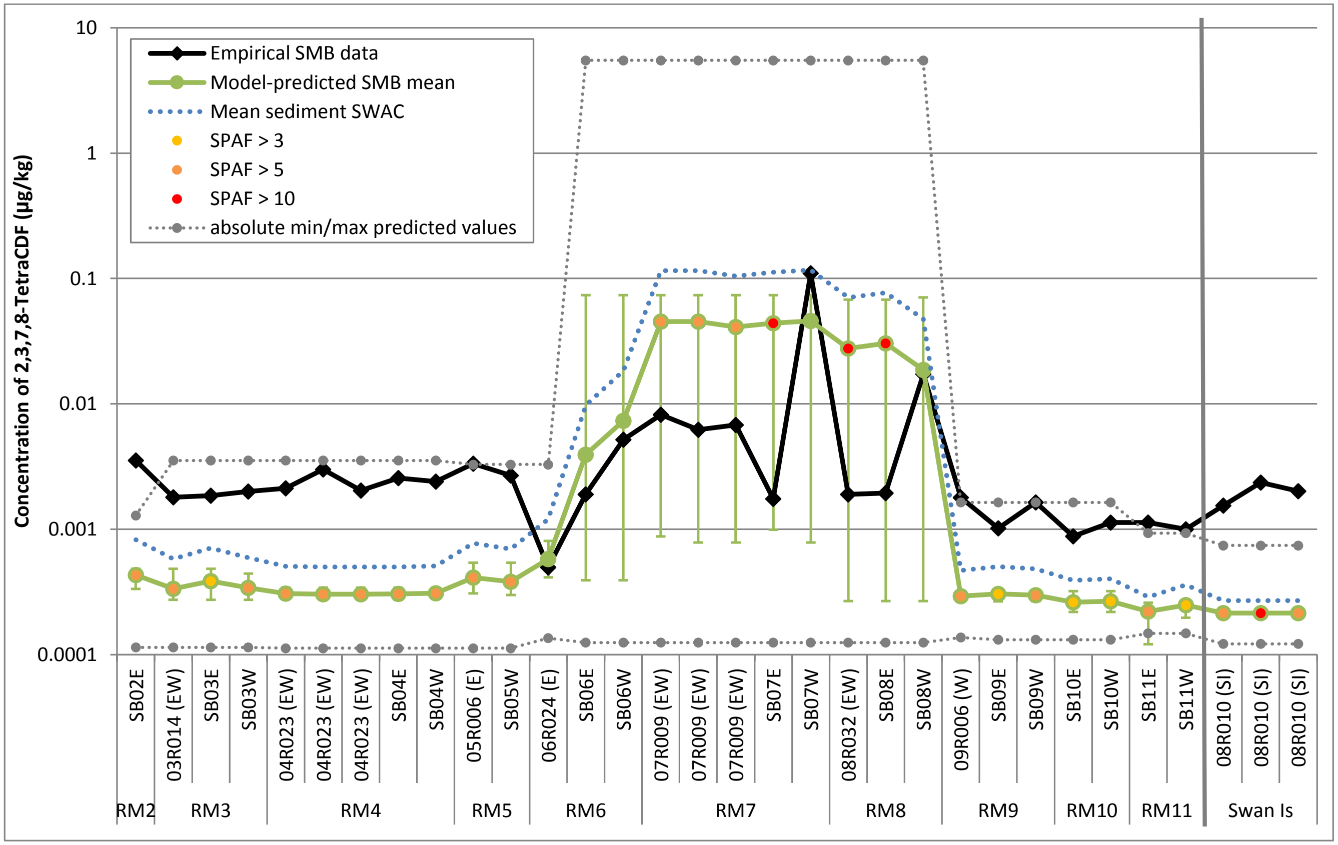


Figure 6-10. Empirical and Model-Predicted Smallmouth Bass Tissue Concentrations for 2,3,7,8-TetraCDF for RM 2 through RM 11 and for Swan Island Lagoon (NEW)

6.3.3 Smaller Spatial Scale Model Application for Sculpin

As was done in Section 5.4.3.4, the calibrated mechanistic model for each dioxin and furan congener was also evaluated on smaller spatial scales for sculpin. Figures 6-11 to 6-15 present model predictions and empirical data for individual sculpin samples by location for each of the congeners (note that two figures are presented for each of the dioxins to show both the Calibration 1 and Calibration 2 results [labeled as figures a and b, respectively]). Predicted and empirical tissue concentrations are on a wet-weight basis, while sediment concentrations are on a dry-weight basis.

As with the model predictions for smallmouth bass for dioxins and furans, the model generally predicted within a factor of 3 compared with the empirical sculpin data based on the mean 0.1-mile-radius SWAC (Figures 6-11 to 6-15). The uncertainty based on the range of sediment concentrations in the exposure areas was often greater for sculpin composite locations where the model did not predict as well, and thus the error bars overlap the empirical sculpin data. This demonstrates that the model works reasonably well when applied at smaller spatial scales for species with home ranges smaller than the site, although the intent of the model was to predict site-wide average concentrations (rather than focus on smaller spatial scales).

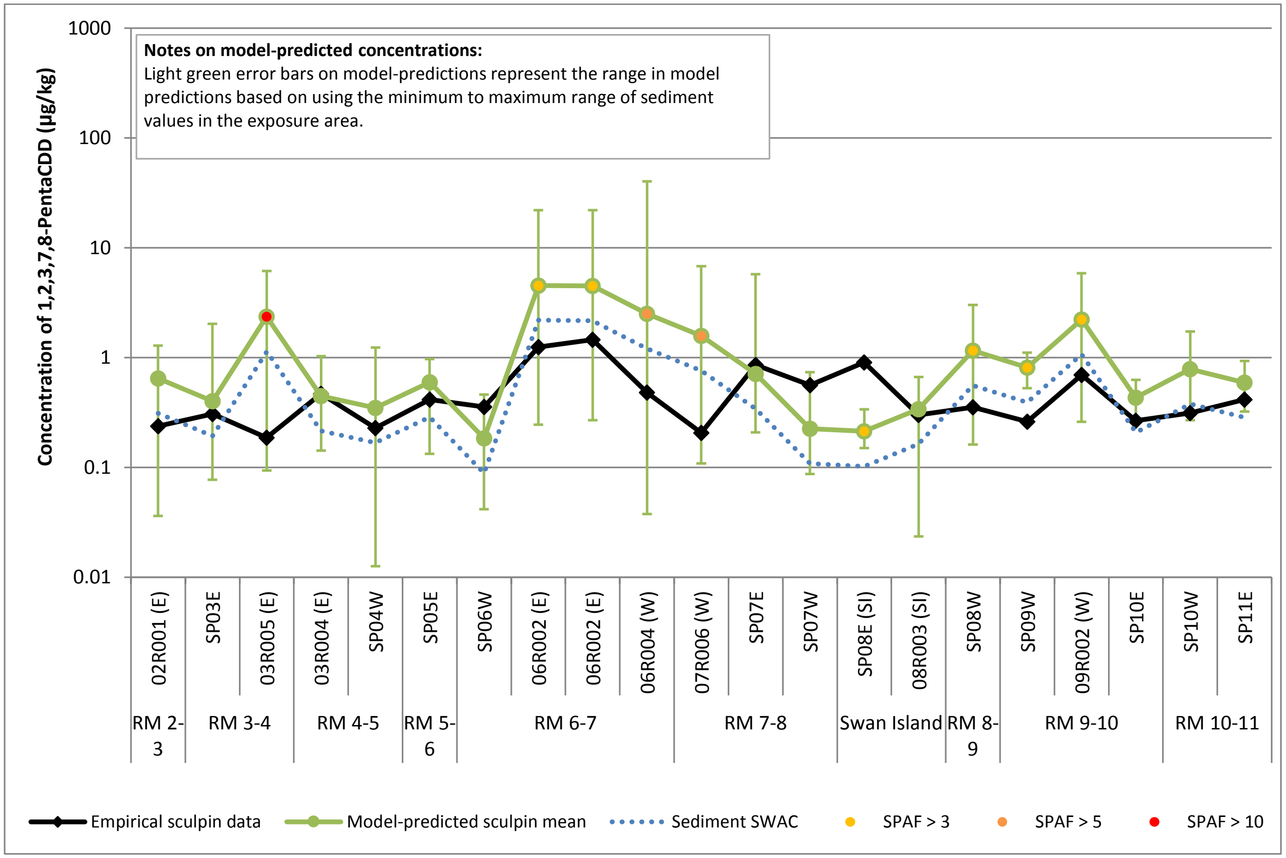


Figure 6-11a. Empirical and Model-Predicted Sculpin Tissue Concentrations for 1,2,3,7,8-PentaCDD for RM 2 through RM 11 using Calibration 1 (NEW)

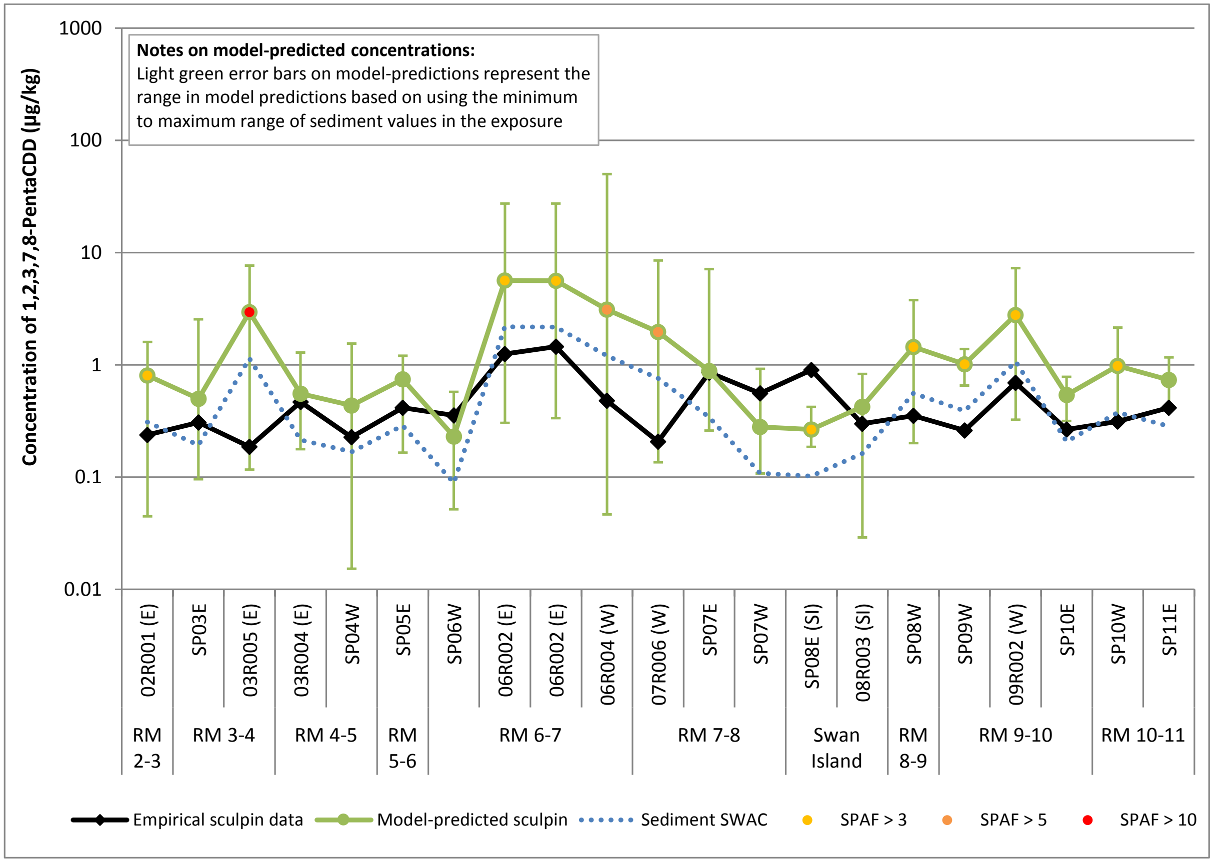


Figure 6-11b. Empirical and Model-Predicted Sculpin Tissue Concentrations for 1,2,3,7,8-PentaCDD for RM 2 through RM 11 using Calibration 2 (NEW)

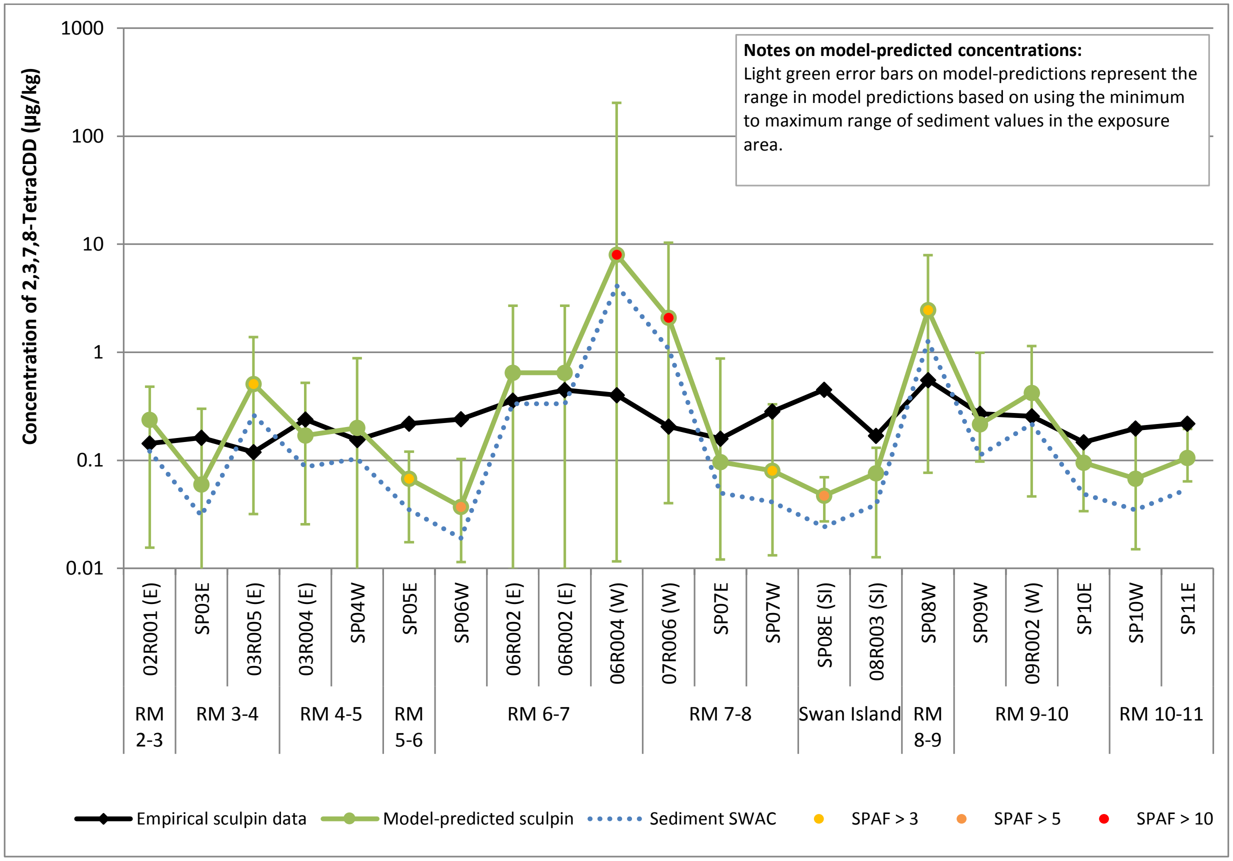


Figure 6-12a. Empirical and Model-Predicted Sculpin Tissue Concentrations for 2,3,7,8-TetraCDD for RM 2 through RM 11 using Calibration 1 (NEW)

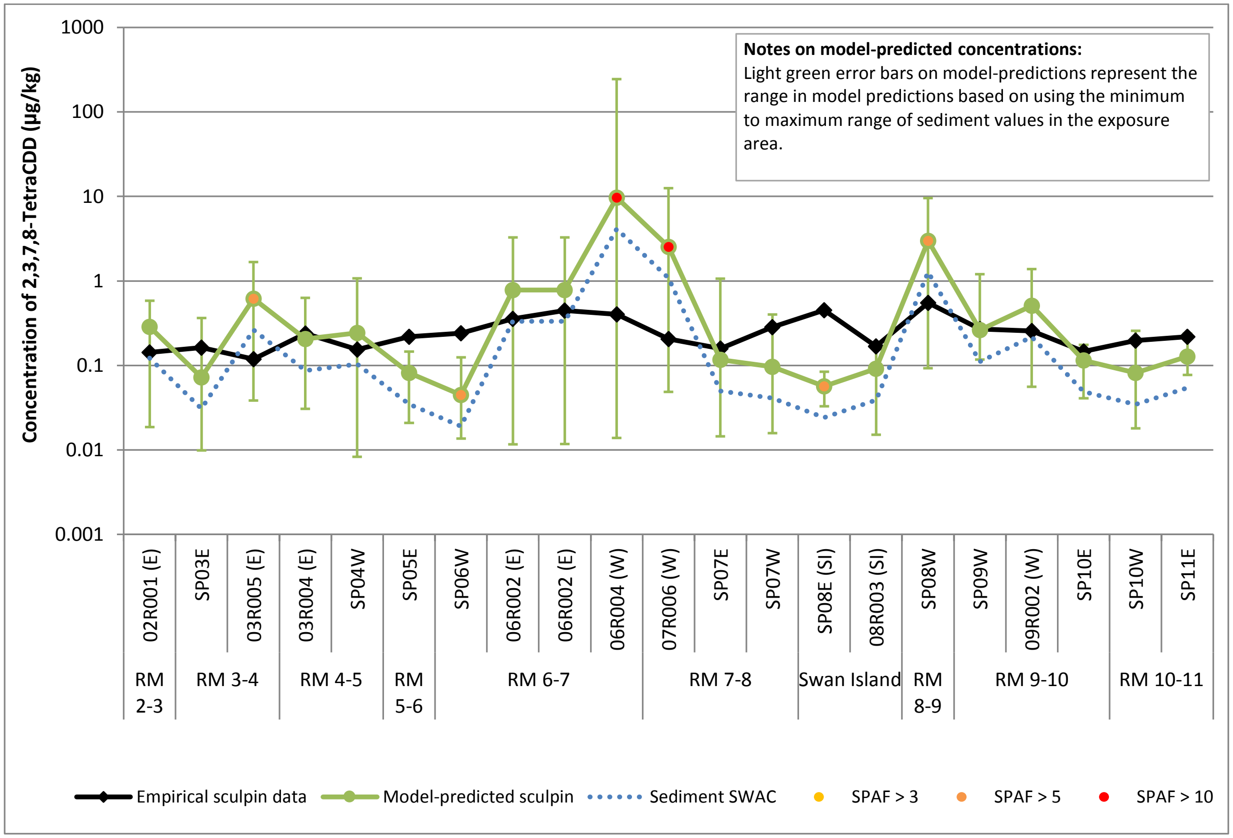


Figure 6-12b. Empirical and Model-Predicted Sculpin Tissue Concentrations for 2,3,7,8-TetraCDD for RM 2 through RM 11 using Calibration 2 (NEW)

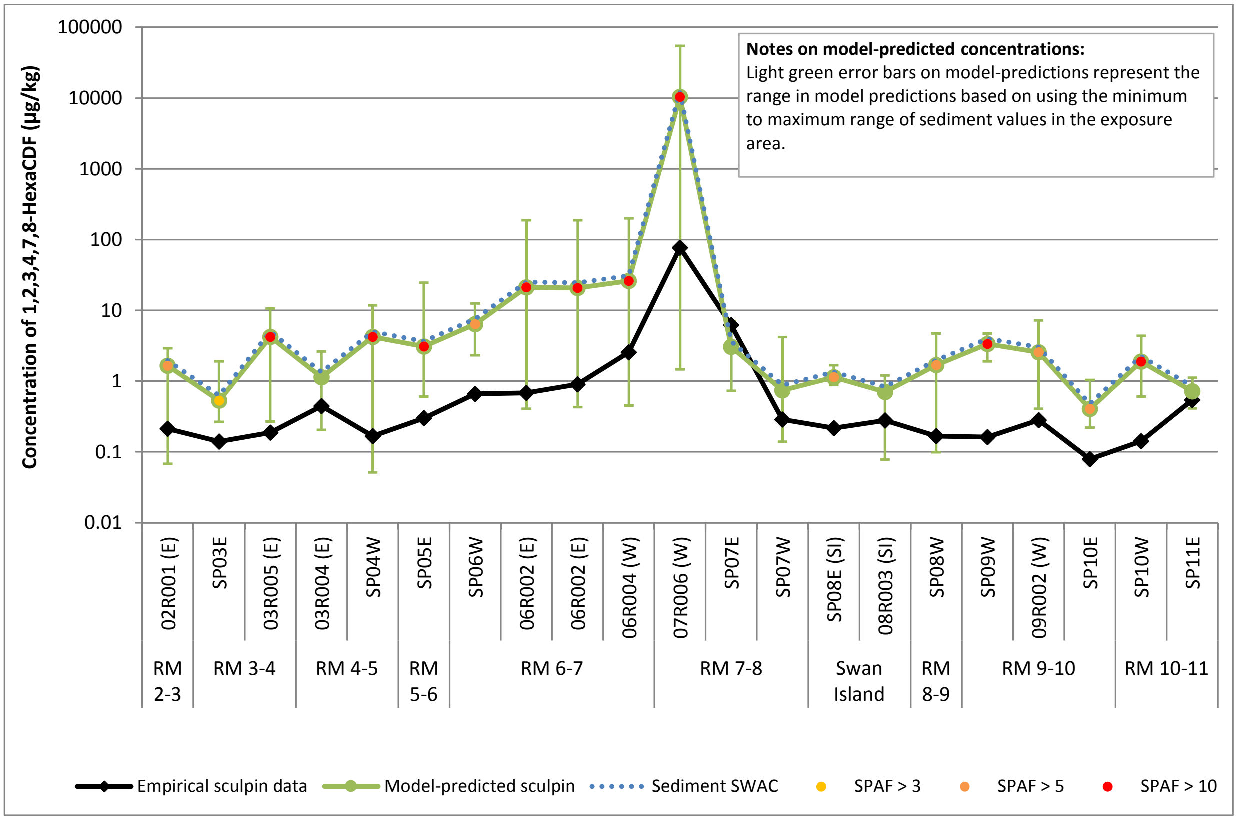


Figure 6-13. Empirical and Model-Predicted Sculpin Tissue Concentrations for 1,2,3,4,7,8-HexaCDF for RM 2 through RM 11 (NEW)

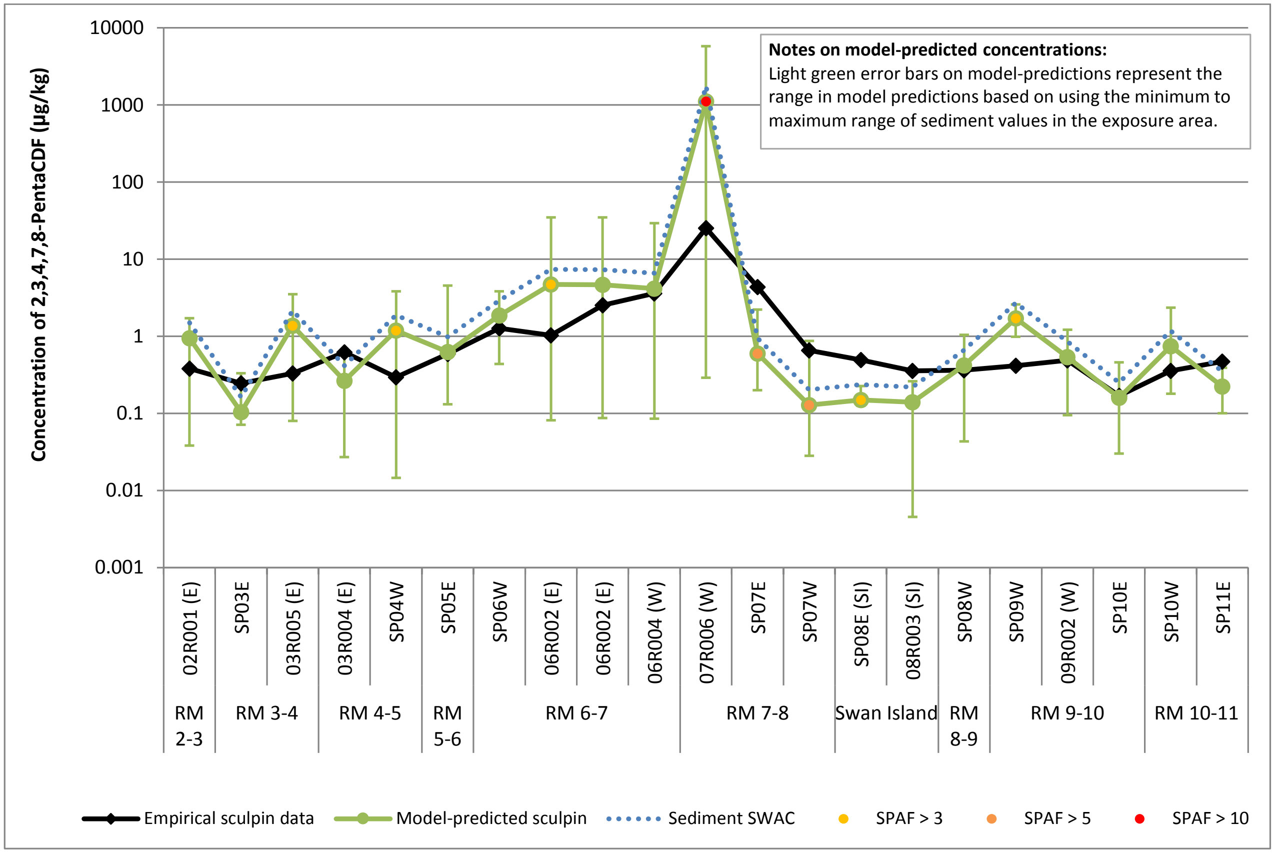


Figure 6-14. Empirical and Model-Predicted Sculpin Tissue Concentrations for 2,3,4,7,8-PentaCDF for RM 2 through RM 11 (NEW)

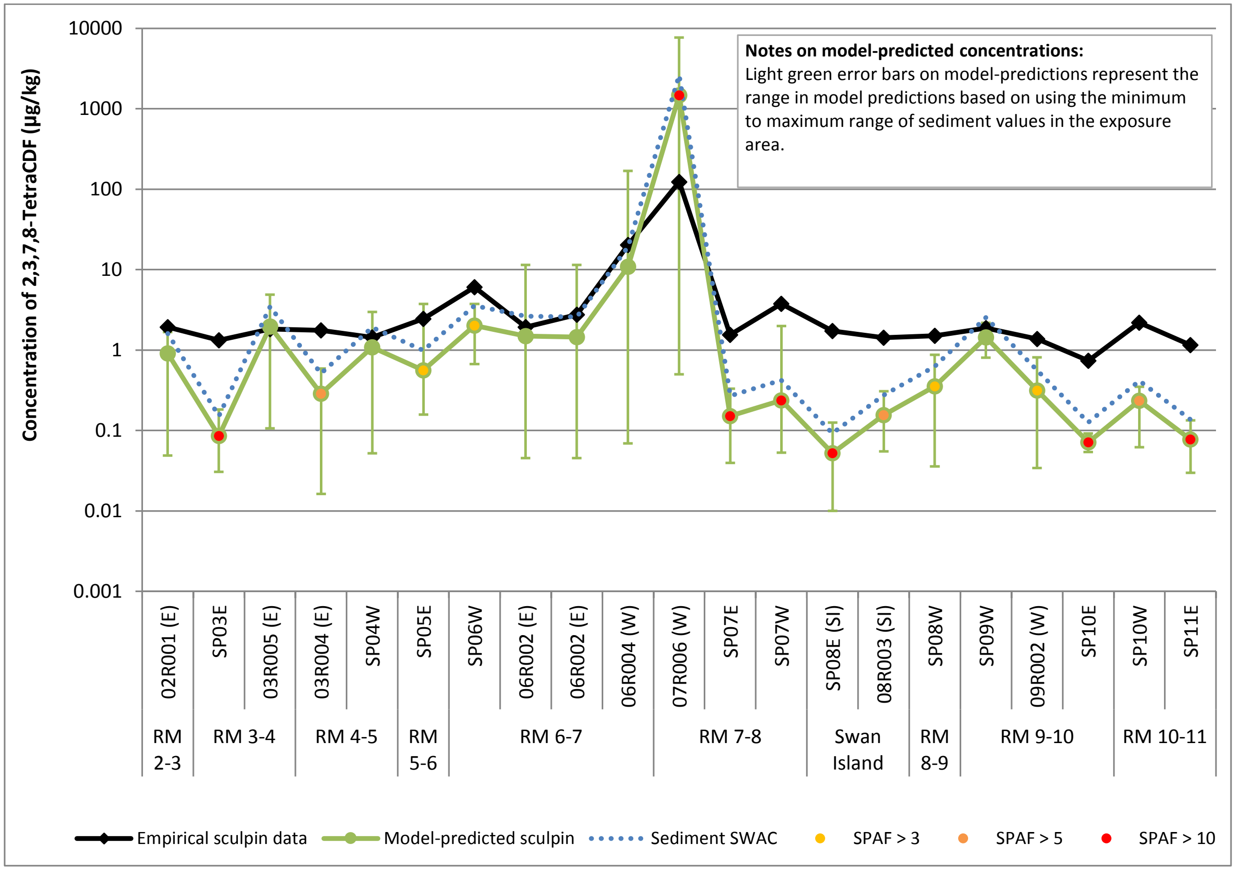


Figure 6-15. Empirical and Model-Predicted Sculpin Tissue Concentrations for 2,3,7,8-TetraCDF for RM 2 through RM 11 (NEW)

6.3.4 Additional Evaluations of the Calibrated Models for Dioxins and Furans

This section presents two additional analyses that were conduced to further evaluate the calibrated models for dioxins and furans. These analyses include the following:

- Water and sediment contribution
- Application of the model for other tissue data

These analyses are discussed in the subsections that follow.

6.3.4.1 Water and Sediment Contribution

As was done in Section 5.5.2 for the other chemicals, Table 6-9 presents a summary of the percent contribution of water to the total chemical burden in tissue (note that together, the sediment and water contributions to the model-predicted tissue concentrations account for 100% of estimated chemical concentration in tissue). As was described in Section 5.5.2, the contribution from water can occur two ways: 1) via direct exposure, and 2) via dietary uptake (the portion of dietary uptake that originated as water contamination lower in the food chain). The contribution from sediment can occur three ways: 1) via direct ingestion of sediment, 2) via porewater ventilation (the chemical concentration in porewater is calculated from the sediment concentration), and 3) via dietary uptake (the portion of dietary uptake that originated as sediment or porewater contamination lower in the food chain). Phytoplankton and zooplankton are not shown in this table because the predicted chemical concentrations for these species are based only on the contribution from the water pathway (100% contribution for all chemicals for these species).

As can be seen in Table 6-9, the percent contribution of water to the model-predicted concentration varied across species and chemicals:

- The percent contribution of water was higher for the two dioxins (based on either calibration) than for the three furans
- Of the furans, 1,2,3,4,7,8-hexaCDF had the highest percent contribution of water; the contributions for the other two furans were generally 2% or lower.
- The percent contribution of water was lower in Calibration 2 for the two dioxins,; largely the result of the lower water concentration.

A detailed discussion of the way that different parameter values (e.g., concentration in water, chemical-specific K_{OW}, and species-specific fraction of porewater ventilation) impact the percent contribution of water to the total body burden was presented in Section 5.5.2.

Table 6-9. Water Contribution to Model-Predicted Tissue Concentrations for Dioxins and Furans (NEW)

	Model Input Values			Percent Contribution from Water Pathway[a]							
Chemical	Sediment (µg/kg dw)	Water (ng/L)	K_{OW}	BIF	BIC	EIC	Sculpin	Largescale Sucker	Carp	Smallmouth Bass	Northern Pikeminnow
Calibration 1											
Dioxins											
1,2,3,7,8-PentaCDD	0.00025	4.3×10^{-6}	6.7	61%	40%	56%	49%	57%	52%	50%	51%
2,3,7,8-TetraCDD	0.0001	2.7×10^{-6}	6.3	65%	46%	62%	56%	61%	59%	57%	58%
Furans											
1,2,3,4,7,8-HexaCDF	0.00271	5.9×10^{-6}	7.0	18%	9%	16%	12%	17%	13%	12%	13%
2,3,4,7,8-PentaCDF	0.0115	3.5×10^{-6}	6.6	3%	1%	3%	2%	2%	2%	2%	2%
2,3,7,8-TetraCDF	0.0168	5.5×10^{-6}	6.3	2%	1%	2%	2%	2%	2%	2%	2%
Calibration 2											
Dioxins											
1,2,3,7,8-PentaCDD	0.00025	1.5×10^{-6}	6.6	34%	18%	30%	25%	30%	27%	25%	26%
2,3,7,8-TetraCDD	0.0001	8.3×10^{-7}	6.3	36%	21%	34%	29%	32%	31%	29%	30%

[a] Water and sediment contribution together account for 100% of the model-predicted chemical concentration in tissue.

BIF – benthic invertebrate filter feeder
BIC – benthic invertebrate consumer
CDD – chlorodibenzo-*p*-dioxin
CDF – chlorodibenzofuran
dw – dry weight
EIC – epibenthic invertebrate consumer
K_{OW} – octanol-water partition coefficient

6.3.4.2 Application of the Model for Other Tissue Data

As has been discussed previously in this document (Section 5.3.1), the mechanistic model is based on a simplified Lower Willamette River food web. Rather than modeling all species, trophic groups were modeled, with a single species used to represent each trophic group in the model (e.g., smallmouth bass represent small piscivorous fish). By using representative species to model an entire trophic group, uncertainties are introduced into model predictions for those species that are not directly modeled. PRGs based on black crappie, brown bullhead, and peamouth were desired, and thus consideration was given to the application of the models for dioxins and furans to these species:

- **Black crappie** – Empirical crappie data were compared with model predictions for sculpin, which were used to represent the forage fish category.
- **Brown bullhead** – Although empirical data were available for brown bullhead, no largescale sucker data were available with which to calibrate the model for benthivorous fish; and thus model performance could not be evaluated for dioxins and furans for this species.
- **Peamouth** – No empirical dioxin or furan data were available for peamouth, and thus model performance could not be evaluated for dioxins and furans for this species.

Table 6-10 presents a comparison of the SPAFs for sculpin (for which the model was calibrated) with the SPAFs resulting from the application of the model to black crappie. As can be seen in this table, the model performed significantly better for sculpin (SPAFs ranging from 1.0 to 3.5) as compared with black crappie (SPAFs ranging from 7.0 to 27). Only four black crappie samples were available, which resulted in a highly uncertain prediction of the average empirical concentration. Moreover, these samples were not collected from areas with high dioxin or furan sediment concentrations, meaning that the available black crappie data do not provide a good representation of the likely site-wide tissue concentration of these chemicals. In comparison, model performance for black crappie for other chemicals (Section 5.6.2) was better (i.e., SPAFs less than 3).

The model predicts other chemical concentrations in black crappie more accurately than furan concentrations because exposure to furans is highly localized relative to the scale of the Study Area. If the problem had been with the model, then the model would have performed poorly for other chemicals as well. It did not. The furan model performance for black crappie is consistent with what one would expect for chemicals with: 1) relatively few localized areas of higher sediment concentrations, and 2) very low background sediment concentrations. The empirical data requirements for calibrating a chemical bioaccumulation model under these conditions, particularly for fish with relatively small exposure areas, are high. In order to accurately estimate SWACs, the sediment data have to be dense enough to accurately estimate the areal fraction of the overall site where the chemical is elevated above background. The fish tissue data have to be dense enough to accurately estimate the fraction of the fish population exposed to elevated sediment chemical concentrations. In the case of furans, these conditions are not met. In the case of black crappie, the high SPAFs simply reflect the fact that apparently none of the collected black crappie were exposed to elevated furans, whereas some of the collected sculpin were. The general conclusions that one can draw from this example are: 1) the black crappie dataset is insufficient to corroborate the furan bioaccumulation model because collected fish were not exposed to elevated sediment furan concentrations, and 2) PRGs set by modeling the 10-mile-long Study Area for chemicals with relatively few, isolated "hot spots" and a low background concentrations are highly uncertain.

Table 6-10. Comparison of Empirical and Model-Predicted Tissue Concentrations for Dioxins and Furans for Species Not Directly Modeled (NEW)

	Sculpin				Black Crappie			
		Tissue Concentration (µg/kg ww)				Tissue Concentration (µg/kg ww)		
Parameter Name	**DF**	**Empirical**	**Model-Predicted[a]**	**SPAF[b]**	**DF**	**Empirical**	**Model-Predicted[a]**	**SPAF[b]**
Calibration 1								
Dioxins								
1,2,3,7,8-PentaCDD	21/21	0.00050	0.0010	+ 2.0	4/4	0.00047	0.0010	+ 2.2
2,3,7,8-TetraCDD	21/21	0.00026	0.00044	+ 1.7	4/4	0.00033	0.00044	+ 1.3
Furans								
1,2,3,4,7,8-HexaCDF	21/21	0.0044	0.0024	- 1.8	4/4	0.00016	0.0024	+ 15
2,3,4,7,8-PentaCDF	21/21	0.0021	0.0074	+ 3.5	4/4	0.00028	0.0074	+ 27
2,3,7,8-TetraCDF	21/21	0.0087	0.0096	+ 1.1	4/4	0.0014	0.0096	+ 7.0
Calibration 2								
Dioxins								
1,2,3,7,8-PentaCDD	21/21	0.00050	0.00086	+ 1.7	4/4	0.00047	0.00086	+ 1.8
2,3,7,8-TetraCDD	21/21	0.00026	0.00033	+ 1.3	4/4	0.00033	0.00033	+ 1.0

[a] Model predictions for brown bullhead were for benthivorous fish (as represented by largescale sucker in the mechanistic model). Model predictions for black crappie were for foraging fish (as represented by sculpin in the mechanistic model). No peamouth data were available for dioxins and furans.

[b] A + or – sign before the SPAF indicates that the model is over-predicting or under-predicting, respectively..

CDD – chlorodibenzo-*p*-dioxin
CDF – chlorodibenzofuran
DF – detection frequency
NA – not applicable
ND – no data
SPAF – species predictive accuracy factor
ww – wet weight

7~~6~~.0 CONCLUSIONS

This report documents attempts to develop bioaccumulation models for all COCs identified in the BERA and BHHRA for the purposes of developing sediment PRGs. Mechanistic modeling is the selected method for developing PRGs because it accounts for water contribution to COC concentrations in tissue, and it is suitable for estimating tissue residue concentrations under projected future conditions, whereas BSAR/Fs should only be used to interpolate within the range of data used to develop them. The mechanistic model describes the bioaccumulation of hydrophobic organic chemicals (Arnot and Gobas 2004). If a non-hydrophobic organic chemical was identified as an ecological COC or human health COC, BSAR/F development for that chemical-species combination was attempted. It was possible to use the mechanistic model for PCBs and several other COCs (i.e. dioxins/furans ~~TEQ~~ and pesticides, including total DDx).

BSARs, which require multiple paired sediment and tissue data, were attempted for numerous COCs for species whose exposure areas are smaller than the Study Area. BSAFs, which are a simple ratio of average tissue to average sediment concentration, were developed only for species with Study Area-wide exposure areas. For the majority of chemical-species combinations for which BSARs were attempted, few BSARs could be developed either because data were insufficient or no model passed the screening criteria. In cases when a BSAR could be developed, the relationship was usually weak (i.e., r^2 was between 0.3 and 0.5). BSAFs for only one chemical were developed; however, there is no significance test for BSAFs since they are simple average concentration ratios. The limited success of the BSAR/F modeling was not a surprising outcome given that the non-hydrophobic organic chemicals are by definition less prone to partition to OC.

The mechanistic model was applied successfully for total PCBs, select dioxin/furan congeners~~TEQ~~, ~~PCB TEQ,~~ and pesticides including total DDx. For all chemicals, the model met or exceeded the stated objectives outlined in this document (i.e., SPAF < 3 for smallmouth bass and < 10 for other species). The calibrated model had SPAFs < 2 for smallmouth bass for all modeled chemicals and generally < 5 for other species-chemical combinations (Section 5.4.1 and Section 6.3). Additionally, the model has been shown to perform well across a variety of chemical types (pesticides, PCBs, and dioxins), species (fish and invertebrates), K_{OW}s, and spatial scales (Study Area-wide and smaller). Additionally, model performance is significantly better than that for the model developed as part of the Round 2 Report because of improvements to the calibration process and better definition of key parameters, due primarily to larger site-specific datasets (Section 5.2).

In conclusion, the bioaccumulation modeling presented in this report is suitable and reliable for calculating sediment PRGs for the Lower Willamette River.

8~~7~~.0 REFERENCES

Arnot JA, Gobas FAPC. 2004. A food web bioaccumulation model for organic chemicals in aquatic ecosystems. Environ Toxicol Chem 23:2343-2355.

Arnot JA, Mackay D, Parkerton TF, Bonnell M. 2008. A database of fish biotransformation rates for organic chemicals. Environ Toxicol Chem 27(11):2263-2270.

Barber MK. 2008. Dietary uptake models used for modeling the bioaccumulation of organic contaminants in fish. Environ Toxicol Chem 27(4):755-777.

Burkhard LP. 2006. Estimation of biota sediment accumulation factor (BSAF) from paired observations of chemical concentrations in biota and sediment. EPA/600/R-06/045. Ecological Risk Assessment Support Center, US Environmental Protection Agency, Cincinnati, OH.

Cunjak RA, Roussel J-M, Gray MA, Dietrich JP, Cartwright DF, Munkittrick KR, Jardine TD. 2005. Using stable isotope analysis with telemetry or mark-recapture data to identify fish movement and foraging. Oecologia 144:636-646.

de Smith M, Goodchild M, Longley P. 2008. Geospatial analysis: a comprehensive guide [online]. Matador, Leicester, UK. Available from: http://www.spatialanalysisonline.com/output/.

EPA. 2006. EPA comments on food web modeling report: evaluating TrophicTrace and the Arnot and Gobas Models for application to the Portland Harbor Superfund Site (November 2005 draft). March 10, 2006. US Environmental Protection Agency, Region 10, Portland, OR.

EPA. 2008a. EPA letter and attachment dated August 8, 2008 to Lower Willamette Group (from E. Blischke and C. Humphrey to J. McKenna and R. Wyatt) regarding Portland Harbor RI/FS: comments on Appendix E - Comprehensive Round 2 Site Characterization and Data Gaps Analysis Report. US Environmental Protection Agency Region 10, Oregon Operations Office, Portland, OR.

EPA. 2008b. EPA letter and attachments dated January 15, 2008 to Lower Willamette Group (from E. Blischke and C. Humphrey to J. McKenna and R. Wyatt) regarding Portland Harbor RI/FS: comments on Comprehensive Round 2 Site Characterization and Data Gaps Analysis Report. US Environmental Protection Agency Region 10, Oregon Operations Office, Portland, OR.

EPA. 2008c. Problem formulation for the Baseline Ecological Risk Assessment at the Portland Harbor Site. Report and letter dated February 15, 2008 to Lower Willamette Group (from E. Blischke and C. Humphrey to J. McKenna and R. Wyatt). US Environmental Protection Agency Region 10, Oregon Operations Office, Portland, OR.

EPA, USACE. 1998. Evaluation of dredged material proposed for discharge in waters of the U.S.- testing manual: Inland Testing Manual. EPA-823-B-98-004. US Environmental Protection Agency and US Army Corps of Engineers, Washington, DC.

Friesen TA, ed. 2005. Biology, behavior, and resources of resident and anadromous fish in the Lower Willamette River. Final report of research, 2000-2004. Prepared for City of Portland. Oregon Department of Fish and Wildlife, Clackamas, OR.

Hill J, Grossman GD. 1987. Home range estimates for three North American stream fishes. Copeia 1986:376-380.

Integral, Windward, Kennedy/Jenks, Anchor, Groundwater Solutions. 2004. Portland Harbor RI/FS programmatic work plan. Prepared for Lower Willamette Group. April 23, 2004. Integral Consulting, Inc., Mercer Island, WA; Windward Environmental LLC, Seattle, WA; Kennedy/Jenks Consultants, Portland, OR; Anchor Environmental, LLC, Seattle, WA; Groundwater Solutions, Inc., Portland, OR.

Integral, Windward, Kennedy/Jenks, Anchor. 2007. Portland Harbor RI/FS: Comprehensive round 2 site characterization summary and data gaps analysis report, plus addenda. IC07-0004. Prepared for Lower Willamette Group. Integral Consulting, Inc., Mercer Island, WA; Windward Environmental LLC, Seattle, WA; Kennedy/Jenks Consultants, Portland, OR; Anchor Environmental, LLC, Portland, OR.

Integral, Windward, Kennedy/Jenks, Anchor QEA. 2011. Portland Harbor RI/FS: Remedial investigation report. IC09-0003. Draft final. Prepared for Lower Willamette Group. August 2011. Integral Consulting, Inc., Mercer Island, WA; Windward Environmental LLC, Seattle, WA; Kennedy/Jenks Consultants, Portland, OR; Anchor QEA, LLC, Portland, OR.

Kennedy/Jenks. 2013. Portland Harbor RI, Appendix F: Baseline human health risk assessment. Final. Prepared for the Lower Willamette Group. March 28, 2013. Kennedy/Jenks Consultants, Portland, OR.

Konwick BJ, Garrison AW, Black MC, Avants JK, Fisk AT. 2006. Bioaccumulation, biotransformation, and metabolite formation of fipronil and chiral legacy pesticides in rainbow trout. Environ Sci Technol 40:2930-2936.

Loonen H, Tonkes M, Parsons JR, Govers HAJ. 1994. Bioconcentration of polychlorinated dibenzo-p-dioxins and polychlorinated dibenzofurans in guppies after aqueous exposure to a complex PCDD/PCDF mixture: relationship with molecular structure. Aqua Tox 30:153-169.

McFarland VA. 1994. Evaluation of field-generated accumulation factors predicting the bioaccumulation potential of sediment-associated PAH compounds. Ph.D. dissertation. Northeast Louisiana University, Monroe, LA. 139 pp.

Morgan MG, Henrion M. 1990. Uncertainty: a guide to dealing with uncertainty in quantitative risk and policy analysis. Cambridge University Press, Cambridge, UK.

Natsumeda T. 1998. Home range of the Japanese fluvial sculpin, *Cottus pollux*, in relation to nocturnal activity patterns. Environ Biol Fish 53:295-301.

Natsumeda T. 1999. Year-round local movements of the Japanese fluvial sculpin, *Cottus pollux* (large egg type), with special reference to the distribution of spawning nests. Ichthyol Res 46(1):43-48.

Natsumeda T. 2001. Space use by the Japanese fluvial sculpin, *Cottus pollux*, related to spatio-temporal limitations in nest resources. Environ Biol Fish 62:393-400.

Neter J, Wasserman W, Kutner MH. 1990. Applied linear statistical models. 3rd ed. IRWIN, Homewood, IL.

Niimi AJ. 1996. Evaluation of PCBs and PCDD/Fs retention by aquatic organisms. Sci Tot Environ 192:123-150.

ODEQ. 2006. Portland Harbor Superfund Site: Models for estimation of chemical distribution and fate in response to remedial alternatives in the Lower Willamette River. Revised working draft, 21 April 2006. Oregon Department of Environmental Quality, Portland, OR.

Opperhuizen A, Sijm DTHM. 1990. Bioaccumulation and biotransformation of polychlorinated dibenzo-p-dioxins and dibenzofurans in fish. Environ Toxicol Chem 9:175-186.

Petty JT, Grossman GD. 2004. Restricted movement by mottled sculpin (Pisces: Cottidae) in a southern Appalachian stream. Freshwat Biol 49:631-645.

Pribyl AL, Vile JS, Friesen TA. 2005. Population structure, movement, habitat use, and diet of resident piscivorous fishes in the Lower Willamette River. In: Friesen TA, ed, Biology, behavior, and resources of resident and anadromous fish in the Lower Willamette River. Final report of research, 2000-2004. Prepared for City of Portland. Oregon Department of Fish and Wildlife, Clackamas, OR, pp 139-183.

Sijm DTHM, Wever H, Opperhuizen A. 1993. Congener-specific biotransformation and bioaccumulation of PCDDs and PCDFs from fly ash in fish. Environ Toxicol Chem 12:1895-1907.

Windward. 2004. Portland Harbor RI/FS. Technical memorandum: evaluating steady-state aquatic food web models for the Portland Harbor Superfund site. WE-04-0002. Draft. Prepared for Lower Willamette Group. Windward Environmental LLC, Seattle, WA.

Windward. 2005. Portland Harbor RI/FS. Food web modeling report: evaluating TrophicTrace and the Arnot and Gobas models for application to the Portland Harbor Superfund Site. WE-05-0009. Draft. Prepared for Lower Willamette Group. Windward Environmental LLC, Seattle, WA.

Windward, Kennedy/Jenks, Integral, Anchor QEA. 2009. Portland Harbor RI/FS. Early preliminary remediation goals. Draft. AQ09-05. March 2, 2009. Windward Environmental LLC; Kennedy/Jenks Consultants; Integral Consulting Inc.; Anchor QEA, LLC, Seattle, WA.

Windward. 2013. Portland Harbor RI/FS, Final Remedial Investigation Report, Appendix G: Baseline ecological risk assessment. Final. Prepared for the Lower Willamette Group. December 16, 2013. Windward Environmental LLC, Seattle, WA.